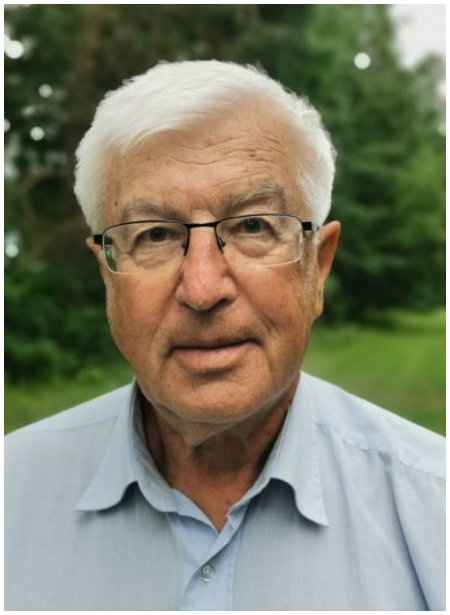


CURRICULUM VITAE

EUGENE KOTOMIN

PERSONAL DETAILS

Name	Eugene KOTOMIN (Jevgenijs Kotomins), PhD, Dr.Sc. in Physics, Dr.habil.phys., Prof., full member of the Latvian Academy of Sciences
Date of birth	September 20, 1949, Vilnius, Lithuanian Republic
Address	Institute of Solid State Physics, University of Latvia, 8 Kengaraga Str., LV-1063 RIGA, Latvia
Phone	371-2999-83-63
E-mail	kotomin@latnet.lv, http://www.cfi.lu.lv/teor/index.html, www.lza.lv/scientists/kotomine.htm
Marital Status	Married, two children

Total citation: 13.000+ ; H-index (Scopus): 58;
560 research papers (2 papers cited more than 200 times, 10 cited more than 100 times). Total 12 review articles, author/editor of 17 books and book chapters, 600 conference Abstracts.

According to a leading academic platform for researchers "research.com" release in 2023, E.Kotomin have been ranked Nr. 1 in Latvia
in the field of (theoretical) chemistry

https://research.com/scientists-rankings/chemistry/lv

EDUCATION

1966-71	BS and MS degrees: Department of Physics, Latvian State University (LSU), 19 Rainis Blvd., Riga LV-1058, Latvia
1973-74	Visiting Fellow, Department of Quantum Chemistry, Leningrad University. Advisor: Prof. R.A. Evarestov
1975	PhD degree: Institute of Physics, The Latvian Academy of Sciences. Advisor: Prof. I. Tale; **Title of Thesis**: "Role of electron tunnelling in radiation-induced defect accumulation and in diffusion-controlled reactions of defects"
1988	Dr.Sc. (Soviet Doctor of Sciences) degree in Solid State Physics; **Title of Thesis**: "Theory of defect accumulation and recombination in ionic crystals controlled by electron tunnelling".
1992	Dr.habil. in Physics, University of Latvia, Riga

ACADEMIC AND PROFESSIONAL EXPERIENCE

1971-74	Engineer and Research Associate, Institute of Solid State Physics, Latvian State University, 8 Kengaraga Str., LV-1063, Riga, Latvia
1975-79	Assistant Professor, Dept. of Semiconductor Physics, Latvian State University
1980-85	Scientist and Senior Scientist at the Institute of Solid State Physics
1986	Senior Visiting Fellow, Dept. of Theoretical Chemistry, Turin University, Italy. Advisor: Prof. C. Pisani
1987-91	General Physics Lecturer and Associate Professor, Dept. of Semiconductor Physics, Latvian State University
1988-present	Head of the laboratory for Theoretical Physics and Computer Modelling; Senior Scientist at the Institute of Solid State Physics, the University of Latvia, Riga
1996-2002	Full Professor at the University of Latvia

PROFESSIONAL ACTIVITIES, FELLOWSHIPS

10.2011	Full Member of the Latvian Academy of Sciences
11.2009	Corresponding Member of the Latvian Academy of Sciences
05-06.1989	Invited Professor, Inorganic Chemistry Dept., University of Turin, Italy
05.1990, 03.1991	Visiting Scientist, University of Bayreuth, Germany

12.1990	Visiting Scientist, Ben-Gurion University, Israel
09.91-02.1992; 03.1999	CCP Fellow at the University of Western Ontario, Canada
10-11.1992	Visiting Scientist, Max-Planck-Institut (MPI) für Metallforschung, Stuttgart
05-06.1993	NUFFIC Fellow, ECN Institute, The Netherlands
11.1993-06.1994	DFG Fellowship at the MPI für Metallforschung, Stuttgart
09.1994-09.1995	Visiting Professor at University of Aarhus, Denmark
07.1996-09.1996	Visiting Scientists at University of Aarhus
09.1997	Visiting Scientist at University of Madrid, Spain, and Western Ontario University, London, Canada
03.1998	Visiting Professor at Tsukuba Science City, Japan
08.1998-08.1999	DFG Visiting Professor at Universität Osnabrück, Germany
09.1999-03.2000	Visiting Scientist at Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany
04.2000-03.2001	DAAD Visiting Professor at Universität Osnabrück, Germany
04.2001-08.2005	Visiting Scientist at Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany
08.2005-07.2007	Visiting Scientist at EC Institute for Transuranium Elements, Karlsruhe, Germany
08.2007-12.2025	Visiting Scientist at Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany
2005-2025	External evaluator of the DOE, NSF and PNNL research projects in the USA, EC ERA-NET, DFG (Germany), Ireland, PAZY foundation, Israel

Member of the organizing committees of the following conferences:

- Quantum Chemistry of Solids; Riga 1985, 1990;
- Radiation Effects in Insulators: (REI-8), Catania, 1995; (REI-9), Tennessee, 1997; (REI-10), Jena, 1999; (REI-11),Lisbon, 2001 ; (REI-12), Brazil, 2003 ; (REI-14), Caen, 2007; (REI-15), Padova, 2009; (REI-16) Beijing, 2011; Helsinki 2013 (REI-17); Versaille 2017 (REI-19); Astana 2019 (REI-20); Madrid 2025 (REI-22)
- European Materials Research Society Meeting, Strasburg, 1995; 2015, 2018; Warsaw, 2012 and 2017; Lille, 2014-2016;

- NATO Advanced Research Workshop on Defects and Surface-Induced Effects in Advanced Perovskites, Riga, August 1999;
- International workshop on Microstructure of Oxide Materials, Osnabrück, June 2000;
- co-director of the NATO school on Computational Materials Science, IlCicco, Italy, September 2001;
- co-director of the NATO school on Radiation Effects in Solids, Erice, Italy, July 2004
- co-organizer of the International workshop on Computational Electrochemistry, Santorini, Greece, September 2004
- co-organizer of the International workshop on First Principles Calculations of Nuclear Fuels, Karlsruhe, Germany, March 2007
- organizer of the International workshop on Ceramic Membranes for Energetics, Riga, Latvia, April 2011
- organizer of the International workshop on Defects in Reducible Oxides (COST Action CM 1104), Riga, Latvia, April 2014

50 Invited talks at the following international conferences, including:

- Radiation Effects in Insulators (REI), Nagoya, 1994 and REI-9, Knoxville, 1997; Caen 2007, REI-14
- NATO Advanced Research Workshop on Computer Modelling of Processes in Solids, Wroclaw, 1996
- Defects in Insulating Materials (ICDIM), Winston-Salem, 1996, Johannesburg, 2000; Santa Fe, 2012
- 2nd International Conference on Excitonic Processes in Condensed Matter, Kurort Gohrisch, Germany, 1996
- Advanced Optical Materials and Devices, Riga, Latvia, 1996
- 1st ABS International Symposium on Metal Oxide Surfaces, Tsukuba, Japan, 1998
- 12 Nordic Symposium on Computer Simulations, Finland, 1998
- European Materials Research Society Meetings, Strasburg, 1995, 1999, 2019
- NATO ARW on Atomistic Aspects of Epitaxial Growth, Corfu, 2001
- 10th International Ceramic Congress, Florence, 2002
- Electronic Structure: Principles and Applications (ESPA-2004), Valladolid, Spain, 15-17 September 2004

- 2 lectures at NATO school on Radiation Physics, Erice, Italy, July 2004
- XNO workshop on nuclear fuels modelling, Tokyo, February 2008
- Baltic Conferences on Functional Materials and Nanotechnology, Riga, 2008, 2009, 2010, 2011
- 5. Baltic Conference on Electrochemistry, Tartu, May 2008
- International Workshop on Ab initio simulations of crystalline solids, Torino, Italy, September 2008
- International Workshop on Fundamentals of Li-based Batteries, Tegersee, Germany, November 2008
- Materials Science and Technology, Pittsburg, USA, October 2009, 2014, Columbus 2011
- 14th International Conference on Radiation Physics and Chemistry of Inorganic Materials, Astana, Kazakhstan, October 2009
- International Symposia on Systems with Fast Ionic Transport (ISSFIT-9,10), Riga, June 2010, Moscow 2012, Kaunas 2016
- CECAM workshop on Actinides: Correlated Electrons and Nuclear Materials, Manchester, UK, June 2010
- Summer school on Ceramic membranes for green chemical production and clean power generation, Valencia, September 2010
- CRYSTAL school on ab initio materials calculations, Torino, Italy, September 2011
- International Conference on Defects in Insulating Materials (ICDIM) Santa Fe, June 2012
- Materials Research Society Meeting, San Francisco, 2013
- International workshop on Electrochemistry, Monterey, USA, June 2014; Ulm 2015
- International School on Electrochemical Energy Conversion and Storage, Stuttgart, 2016
- Schools-conferences on "Atomistic Simulations of Functional Materials" (Moscow, Russia, 2014-2018)
- 232st Electrochemical Society Meeting, New Orleans, USA, 2017
- 21st International Conference on Solid State Ionics, Padua, Italy, 2017
- European Conference on defects in Insulating Materials (EURODIM), (Bydgoszcz, Poland, 8-13 July 2018).
- The 18th Israel Materials Engineering Conference IMEC-18 (Dead Sea, Israel, February 2018).

- American Ceramic Society meeting (Orlando, January 2020)

  Member of the:

  - Full Member of the Latvian Academy of Sciences since 2011
  - American Ceramic Society since 2014
  - Americal Chemical Society since 2020
  - New York Academy of Sciences, 1992-95
  - American Physical Society, 1992-95
  - Materials Research Society, 1992-present
  - American Geophysical Union, 1995-present
  - Association of Latvian Scientists, 1991-present
  - Council for Dissertations of Latvian University, 1987-91
  - Editorial Advisory Board of the Journal *Diffusion and Defect Data*

RESEARCH SUPPORT AND AGENCY

1992	International Science Foundation (ISF) grant
1992	NATO collaborative grant on Defects in Oxides
1993, 1994,1997	ISF (Soros) travel grants for International conferences
1994-96	Two-year ISF research grant
1994-96	European Community Human Capital and Mobility (HCM) Network Grant on *Polarons and Bipolarons in New Materials*
1994-96	European Community HCM Network Grant on *Large Scale Computer Simulations of Solids*
1996-98	Volkswagen research grant (Freie Universität Berlin, Germany)
1999-2000	NATO research grant for senior visitors (Aarhus University, Denmark)
1999-2000	British-Latvian UK Royal Society Joint grant (University College London)
1999-2003	Swedish-Latvian Joint research grants with Uppsala University
2001-2004	Networking grant in the framework of the EC Excellence Center for Materials Research and Technology, CAMART

2001-2003	NATO collaborative grant on Defects in Perovskites, Osnabrueck University, Germany
2003-2006	Research grant of German-Israeli Foundation: MPI,Stuttgart– Technion, Israel
2002-2005	Member of the European Network Psi-k2 on Atomistic Materials Design
2005-2007	NSF collaborative grant on Reactivity of Oxide Surfaces with NRSEC Northwestern University, USA
2005-2007; 2010-2012; 2017-2020	Three projects of the German-Israel Foundation (GIF) on new materials for solid oxide fuel cells
2006-2010	Three service contracts on ab initio modelling of nuclear fuels with JRC-ITU, Karlsruhe, Germany
2006-2014	Euratom-Latvia project on modeling of ODS steel formation as reactor materials, Brussels, Belgium
2007-2008	Actinet: EC Euratom Network on He modelling in nuclear fuels
2008-2011	EC FP7 Project F-Bridge on nuclear fuel modelling
2009-2012	EC FP7 Project NASA-OTM on ceramic permeation membrane modelling
2008-2012	ERA-NET project MATERA on materials for resistive switching
2013-2018	EC FP7 Project GREEN-CC on advanced ceramic membranes
2012-2015	EC COST Action CM 1104 on Reducible Oxides
20015-2019	Eurofusion project on Functional optical materials
2014-2018	Russian Science Foundation project 14-43-00052 on large scale advanced materials modelling
2015-2017	Eurofusion Enebling Research Project on X-ray Absorption Spectroscopy and atomic-scale modelling of ODS steels
2016-2019	M-ERA-NET project HarvEnPiez on Innovative nano-materials and architectures for integrated piezoelectric energy harvesting applications
2018-2019	Bilateral Latvia-Ukraine project on perovskite surface reactivity

2019-2025	EC COST Action OC-2018-2-23544 Computational materials sciences for efficient water splitting with nanocrystals from abundant elements
2019-2022	M-ERA-NET project Sun2Chem on Engineering of perovskite photocatalysts for sunlight-driven hydrogen evolution from water splitting
2024-2026	M-ERA-NET project HetCat on Heterogeneous catalysis applied to sunlight-driven hydrogen evolution
2025-2027	M-ERA-NET project GRIPHUS (GReen Innovative PHotocatalytic systems for CO2 Utilization to produce e-fuelS)
2024-2026	Development of new advanced phosphors for lighting and non-contact optical thermometry Latvian Council of Science (LZP grant 2023-0063)

AWARDS

1997 Fridrich Cander prize in physics of the Latvian Academy of Sciences

2023 Edgar Silinsh prize in physics of the Latvian Academy of Sciences

Reviewer for more than 40 basic research journals, including MDPI journals, Physical Review Letters, Physical Review B and E, Nature Materials, Journal of Nuclear Materials, Nuclear Instruments and Methods B, Solid State Ionics, Surface Science, Physical Chemistry Chemical Physics, Physica Status Solidi, Physica B, J Luminescence, Chemistry of Materials, J Physical Chemistry J Physics: Condensed Matter, Solid State Communications, Chemical Physics, Philos. Magazin, Applied Physics Letters, J. Materials Research, etc.

TEACHING EXPERIENCE

I lectured at undergraduate/graduate levels during five years as Assistant and Associate Professor, and four years as Lecturer at the University of Latvia giving courses in "General Physics", "Quantum Chemistry of Solids", "Theory of Defects in Solids", "Theoretical Characterization of Bulk and Surface Defects in Solids".

As a Visiting Professor, I gave at University of Aarhus in 1995 a PhD course entitled "Static and Dynamic Properties of Defects in Solids" as well as a course on "Defects in Solids" at Osnabrück University in 1998/1999. In 2000-2001, serving as DAAD and DFG invited professor, I gave several courses of lectures in Osnabrück University and later, in 2008, 2009, 2012, 2013, 2014 in Astana Eurasian University (Kazakhstan) on "Computational Methods and Modelling of Advanced Materials".

I have supervised 20 BS theses, 15 MS theses and 8 PhD theses, at the University of Latvia and Max Planck Institute in Stuttgart, Germany.

PUBLICATIONS

Author/co-author of 17 books and chapters, 12 review articles, 560 refereed papers (see attached list of publications).

RESEARCH INTERESTS (in brief)

My recent scientific activities are concerned with the **computational materials science** – interdisciplinary field including condensed matter physics and chemistry, *ab initio* atomic and electronic structure calculations of (mainly oxide) materials, defects therein, quantum chemistry of defective solids, surfaces, and interfaces. In recent years I focused on atomistic understanding of processes at the surfaces of cathodes of solid oxide fuel cells and permeation membranes in order to improve their performance, see e.g. chapter 6 in a book *Computational approaches to energy materials* (eds. A.Walsh, A. Sokol, C.R.A. Catlow, Wiley, 2013).
My research interests include also theory of radiation-induced effects and defects in solids, kinetics of bimolecular reactions with a focus on self-organization phenomena. In cooperation with Prof. V.Kuzovkov, I developed theory of *fluctuation-controlled kinetics of bimolecular chemical reactions* which calls into question the standard criteria generally accepted in synergetics. These results are summarized in our book – E.A. Kotomin and V.N. Kuzovkov, *Modern Aspects of Diffusion- Controlled Reactions*, Elsevier, 1996.

My current research activities are focused on: (i) Functional materials and devices for new energy applications including fussion reactors, solid oxide fuel cells (SOFC), batteries, sensors; (ii) Nanomaterials and confinement effects in advanced perovskites; (iii) Defects and surface-related processes in advanced complex oxides and nitrides; (iv) Physics and chemistry of actinides and nuclear fuels, new functional materials for fusion and fission reactors; (v) Radiation physics and chemistry, self-organization in non-equilibrium systems.

In our research I combine analytical methods with large-scale computer modelling based on the first-principles approaches and kinetic Monte Carlo method.

Most of my diverse interests are fueled by international collaboration such as Max Planck Institute, Stuttgart, Germany (Prof. J. Maier, 'Properties of Perovskite Surfaces'), University of Maryland (Prof. M. Kuklja, 'First-principles modeling of Solid Oxide Fuel Cells'), Turin University, Italy (Prof. R. Dovesi, 'LCAO hybrid Calculations of Solids, Surfaces and Interfaces'), Center of Nanotechnology, University Colledge London, UK (Prof. A.L.Shluger, 'Reducible oxide surfaces'), St.Petersburg University, Russia (Prof. R.A. Evarestov, 'Large-scale Parallel Calculations of Defects and Advanced Perovskite Surfaces') and Juelich Research Center, Germany (Prof. R.Waser, Dr R.Dittmann, 'Materials for resistive switching' and Dr W.Meulenberg 'Advanced permeation membranes').

LIST OF REFEREED PAPERS OF E.A. KOTOMIN

Books and book chapters

1. Evarestov R.A., Kotomin E.A., Ermoshkin A.N. *Molecular models of point defects in wide-gap solids.* -Riga: Zinatne, 1983. -287p.

2. Kantorovich L.N., Kotomin E.A., Kuzovkov V.N., Tale I.A., Shluger A.L., Zakis Yu.R. *Models of defect processes in wide-gap solids.* -Riga: Zinatne, 1991. -320p.

3. Kotomin E.A. and Kuzovkov V.N. *Modern Aspects of Diffusion-Controlled Processes: Cooperative Phenomena in Bimolecular Reactions*, North Holland, Elsevier Publ. (vol. **34** in a series of *Comprehensive Chemical Kinetics*),1996.620 p.

4. Catlow C.R.A. and Kotomin E.A. (eds.) Computational Materials Science, IOS press, Amsterdam, Berlin, Oxford,Tokyo, Washington,DC, 2003, 420 pp. (NATO Science series III: Computer and Systems Sciences, vol. 187).

5. Sickafus K. and Kotomin E.A. (eds.). Radiation Effects in Solids, 2006, NATO ASI Science Series II. Physics, Chemistry and Mathematics, Vol. 235.

6. Kuzovkov V.N., Kotomin E.A., Zvejnieks G., Li K.D., Ding T.H., Wang L.M. Void Superlattice Formation in Electron Irradiated Insulating Materials.– Chapter 11 in: Advances in Materials Science Research, vol. 2, 2011, pp. 191-216 (Nova Science Publishers, ed. Maryann C. Wythers).

7. Heifets E., Kotomin E.A., Mastrikov Yu., Piskunov S., and Maier J. Chapter in: Thermodynamics of ABO_3 perovskite surfaces. – In: Thermodynamics-Interaction studies - Solids, liquids and gases (InTech Open Access Publishers), 2011, p. 491-518.

8. Zhukovskii Yu.F., Bocharov D., Gryaznov D., and Kotomin E.A., First Principles Simulations on Surface Properties and Oxidation of Nitride Nuclear Fuels. - Chapter in book: Advances in Nuclear Fuel (Ed. Shripad T. Revankar, InTech Open Acess Publishers), 2012, p. 95-122

9. Zhukovskii Yu.F., Kotomin E.A., Piskunov S., and Bellucci S., CNT arrays grown upon catalytic nickel particles as applied in the nanoelectronic devices: Ab initio simulation of growth mechanism. - Proc. NATO ARW Nanodevices and Nanomaterials for Ecological Security (Eds. Yuri N. Shunin and Arnold E. Kiv; Springer: Dordrecht, 2012), p. 101-114.

10. Gopejenko A., Zhukovskii Yu.F., Vladimirov P.V., Kotomin E.A., and Moeslang A. Interaction between oxygen and yttrium impurity atoms as well as vacancies in fcc iron lattice: Ab initio modeling. - Proc. NATO ARW Nanodevices and Nanomaterials for Ecological Security (Eds. Yuri N. Shunin and Arnold E. Kiv; Springer: Dordrecht, 2012), p. 149-160

11. Kotomin E.A., Merkle R., Mastrikov Yu.A., Kuklja M.M., and Maier J. — Energy Conversion: Solid Oxide Fuel Cells. –First-Principles Modeling of Elementary Processes. Chapter 6 in the book: "Computational Approaches to Energy Materials" (eds. A.Walsch, A.Sokol, C.R.A. Catlow, Wiley, 2013).

12. Sobolev N., Bernas H., Kotomin E.A. and Nordlund K. (eds.) Defect-induced effects in nanomaterials, Proceedings of Symposium L of the Fall EMRS conference (Warsaw, 2012)– Phys. Stat. Solidi B 250, No 4, 2013.

13. Djurabekova F., Kotomin E.A., Ridgway M., Sobolev N. (eds.) Defect-induced effects in nanomaterials, Proceedings of Symposium E of the Spring EMRS conference (Lille, 2014)– Phys. Stat. Solidi C 12, No 1-2, 2015.

14. Costantini J-M., Trautman C., Weber W., Kotomin E.A. (eds.) Basic Research on Ionic Covalent Materials for Nuclear Applications, Proceedings of Symposium G of the Spring EMRS conference (Lille, 2015) – Nucl. Instr. Meth. B 374,1 (2015).

15. Popov A.I., Lushchik A., Kotomin E.A. Low temperature radiation effects in wide gap materials (eds.) – In: Low Temperature Physics (Fizika nizkih temperatur, 2016, v. 42, N 7, pp. 687-688.

16. Arrigoni M., Kotomin E.A., Maier J., Large Scale Modeling of Defects in Advanced Oxides: Oxygen Vacancies in BaZrO3 Crystals. - Chapter in a book: W. Nagel et al. (eds.) High Performance Computing in Science and Engineering, (Springer, Switzerland), 2016, p. 187-198.

17. Kotomin E.A., Sobolev N., Djurabekova F., Zhang Y., Ridgway M. (eds.) Defect-induced effects in nanomaterials, Proceedings of Symposium BB of the Spring EMRS conference (Lille, 2016)– Phys. Stat. Solidi C 13, 697, 2016; Phys. Stat. Solidi B 253, 2091, 2016

18. Sobolev N., Djurabekova F., Kotomin E.A.,. (eds.) Defect-induced effects in nanomaterials, Proceedings of Symposium K of the Spring EMRS conference (Strasburg 2018)– Phys. Stat. Solidi B 256, 1900181, 2018

Review Articles

1. Doktorov A.B., Kotomin E.A. Theory of Tunnelling Recombination of Defects Stimulated by Their Motion. (I). General formalism. -Phys. Stat. Solidi (b), 1982, **114**, No.1, p.9-14.

2. Kotomin E.A., Doktorov A.V. Theory of Tunnelling Recombination of Defects Stimulated by Their Motion. (II). Three Recombination Mechanisms. -Phys. Stat. Solidi (b), 1982, **114**, No.2, p.287-318.

3. Kalnin Yu.H., Kotomin E.A. Radiation-induced aggregation of immobile Frenkel defects in solids. -Probl. of atom. Sci. and techn., Kharkov phys.-techn. Inst., **20**, 1984, p.18-34.

4. Kuzovkov V.N., Kotomin E.A. Kinetics of bimolecular reactions in condensed media. -Rep. on Progr. in Physics, 1988, **51**, No.12, p.1479-1524.

5. Millers D.K., Grigorjeva L.G., Kotomin E.A., Artjushenko V.G. Butvina L.N. Radiation-induced processes in crystals and fibers made of silver halides. Latv.St.Univ. Preprint. 1988. P.70.

6. Vinetsky V.L., Kalnin Yu.R., Kotomin E.A., Ovchinnikov A.A. Radiation-induced Frenkel defect aggregation in solids. -Sov.phys.-uspekhi, 1990, **33**, No.10, p.793-811.

7. Kotomin E.A., Kuzovkov V.A. Phenomenological theory of the recombination and accumulation kinetics of radiation defects in ionic solids. -Rept.Progr.Phys., 1992, **55**, p.2079-2202.

8. Eglitis R., Kotomin E.A., Borstel G. Large scale computer modeling of point defects, polarons and pervoskite solid solutions. - Defects and Diffusion Forum, 2004, **226-228**, p. 169-180.

9. Zhukovskii Yu., Kotomin E.A., Evarestov R.A., Ellis D.E. Periodic Models in Quantum Chemical Simulations of F Centers in Crystalline Metal Oxides. - Int. J. Quantum Chem., 2007, **107**, p.2956-2985.

10. Kotomin E.A. and Popov A.I. The kinetics of radiation-induced point defect aggregation and metallic colloid formation in ionic solids. In: Radiation Effects in Solids, NATO ASI Science Series II. Physics, Chemistry and Mathematics (Eds. K. Sikafus and E.A. Kotomin), Vol. **235**, p. 153-192.

11. Wang L., Merkle R., Mastrikov Yu., Kotomin E.A., Maier J. Oxygen exchange kinetics on solid oxide fuel cell cathode materials-general trends and their mechanistic interpretation. - J. Mater. Res.,2012, **27**, p.2000-2008.

12. Kuklja M.M., Kotomin E.A., Merkle R., Mastrikov Yu.A., and Maier J., Combined theoretical and experimental analysis of processes determining cathode performance in solid oxide fuel cells. - Phys. Chem. Chem. Phys., Perspective, 2013, **15**, p. 5443-5471.

Papers

1974

13. Fabrikant I., Kotomin E.A. Theory of diffusion-controlled tunnelling recombination (I.) -In: Electronic and ionic processes in ionic crystals. Riga: Latv.Univ.press, 1974, **2**, p.78-92.

14. Kotomin E.A. Theory of diffusion-controlled tunnelling recombination. (II.) -In: Electronic and ionic processes in ionic crystals. Riga: Latv.Univ.press, 1974, **2**, p.93-107.

15. Kotomin E.A., Fabrikant I. Theory of diffusion-controlled tunnelling recombination. (I-III.) -In: Electronic and ionic processes in ionic crystals. -Riga: Latv.Univ.press, 1974, **2**, p.78-123.

16. Tale I.A., Millers D.K., Kotomin E.A. A role tunnelling recombination in low-temperature F centre accumulation. -In: Electronic and ionic processes in ionic crystals. Riga: Latv. Univ. press, 1974, **2**, p.43-51.

1975

17. Kotomin E.A., Fabrikant I.I. Theory of Diffusion-Limited Recombination of Donor-Acceptor Pairs. -J.Luminescence, 1975, **9**, No.6, p.502-513.

18. Ermoshkin A.N., Kotomin E.A., Evarestov R.A. Molecular cluster approach to magnesium and calcium oxide crystals. -Phys. Stat. Solidi (b), 1975, **72**, p.787-798.

19. Millers D.K., Tale I.A., Kotomin E.A. General approach for discribing processes of radiation defect accumulation and annealing in ionic solids. Riga: Latv.Univ.press, 1975, **4**, p.24-72.

20. Tale I.A., Millers D.K., Kotomin E.A. Role of Tunnelling Recombination in Radiation-Induced F Centre Creation in Alkali Halide Crystals. -J.Phys.C: Sol. St. Phys., 1975, **8**, p.2366-2375

21. Plotnikov O.V., Kotomin E.A. Use of consecutive eliminations for the decomposition of complicated ESR spectra.-Sov.J. Appl. Spectr., 1975, No.2, p.79.

1976

22. Ermoshkin A.N., Evarestov R.A., Kotomin E.A. Molecular cluster approach to magnesium oxide crystals. (II). F^+ and F centres. -Phys. Stat. Solidi (b), 1976, **73**, p.81-86.

23. Evarestov R.A., Ermoshkin A.N., Kotomin E.A. Molecular cluster approach to magnesium and calcium oxide crystals. (III). Charge distribution analysis of some hole centres. -Phys. Stat. solidi (b), 1976, **74**, p.483-486.

1977

24. Kotomin E.A. Cirulis Ya.P., Tale I.A. A novel method of decomposition of complex spectra into elementary bands. -Proc. Latv.Univ., 1977, **160**, p.93-123.

25. Kotomin E.A., Fabrikant I.I. Theory of diffusion-Controlled Tunnelling Recombination Incorporating Annihilation and Coulomb Interaction. -J.Phys.C: Sol.St.Phys., 1977, **10**, p.4931-4937.

26. Kotomin E.A., Fabrikant I.I., Tale I.A. Temperature dependence of F centre accumulation efficiency in doped alkali halides. -J.Phys.C: Sol.St.Phys., 1977, **10**, p.2903-2914.

27. Fabrikant I.I., Kotomin E.A. Variational estimates of the quasi- steady-state radius of diffusion-controlled tunnelling recombination incorporating annihilation and Coulomb interaction. -In: Electronic and ionic processes in ionic crystals. Riga: Latv.Univ.press, 1977, **6**, p.39-56.

1978

28. Tale I.A., Kotomin E.A. Tunnelling phenomena. -Science and Technics (Riga), 1978, No.1, p.14-18.

1979

29. Shluger A.L., Kotomin E.A., Dzelme Yu.R. Quantum Chemical Calculations of Electronic, Hole Centres and Surface of NaCl Crystal. (I). -Phys. Stat. Solidi (b), 1979, **96**, No.1, p.91-97.

30. Shluger A.L., Kotomin E.A., Dzelme Yu.R., Ermoshkin A.N. On the semiempirical calculations of electronic structure of perfect and defective alkali halide crystals. -Proc.Latv.Aca. Sci., 1979, No.3, p.116-118.

31. Kotomin E.A., Fabrikant I.I. Efficiency of F centre accumulation in ionic crystals. -Proc.Latv.Aca.Sci., 1979, No.1, p.53-59.

32. Kotomin E.A., Fabrikant I.I. Estimate of quasi-steady recombination radius of defects incorporating tunnelling and elastic interaction. -Proc.Latv.Aca.Sci., 1979, No.3, p.76-83.

1980

33. Kotomin E.A., Shluger A.L., Dzelme Yu.R. Quantum Chemical Calculations of Electron, Hole Centres and Surface of NaCl Crystal. (II). -Phys. Stat. Solidi (b), 1980, **98**, No.2, p.427-433.

34. Kotomin E.A., Fabrikant I.I. Influence of Defect Interaction Upon Their Recombination in Alkali Halides. (I). -Radiat. Effects, 1980, **46**, No.1, p.85-90.

35. Kotomin E.A., Fabrikant I.I. Influence of Defect Interaction Upon Their Recombination in Alkali Halides. (II). -Radiat. Effects, 1980, **46**, No.1, p.91-96.

36. Kuzovkov V.N., Kotomin E.A. Generalized theory of diffusion- controlled defect annealing. -J.Phys.C: Sol.St.Phys., 1980, **13**, No.21, p.L499-L502.

37. Kotomin E.A., Chernov A.S. The temperature dependence of the F centre accumulation efficiency in alkali halides. -Sov.phys. - Solid State, 1980, **22**, No.5, p.1515-1517.

38. Kuzovkov V.N., Kotomin E.A. Formation of clusters of radiation defects. I. Accumulation kinetics of immobile defects. -In: Physics of phase transitions. Riga: Latv.Univ.press, 1980, p.132-146.

39. Kotomin E.A., Kuzovkov V.N. Formation of clusters of radiation defects. II. Mobile defects. -In: Physics of phase transitions. Riga: Latv.Univ.press, 1980, p.132-146.

40. Kotomin E.A., Valdats G.A. Computer simulation of low-temperature F centre accumulation restricted by tunnelling recombination. -In: Electronic and ionic processes in ionic crystals. Riga: Latv.Univ.press, 1980, **8**, p.58-74.

41. Kotomin E.A., Shluger A.L., Ermoshkin A.N., Dzelme Yu. Quantum-chemical calculations of NaF, NaCl crystals and F-centers in their bulk and on the surface. -In: Electronic and ionic processes in ionic crystals. Riga: Latv.Univ.press, 1980, **8**, p.58-74.

1981

42. Kuzovkov V.N., Kotomin E.A. Kinetics of Defect Accumulation and Recombination. (I). General Formalism. -Phys. Stat. Solidi (b), 1981, **105**, No.2, p.789-801.

43. Kotomin E.A. Kuzovkov V.N. Kinetics of Defect Accumulation and Recombination. (II). Diffusion-Controlled Annihilation. -Phys. Stat. Solidi (b), 1981, **108**, No.1, p.37-44.

44. Kotomin E.A., Kuzovkov V.N. Radiation-Induced Aggregation of Immobile Defects. -Sol.St.Comm., 1981, **39**, p.351-354.

45. Ermoshkin A.N., Kotomin E.A., Evarestov R.A. Semiempirical Calculations of the Impurity Level Positions with Respect to the Perfect Crystal Bands. -Phys. Stat. Solidi (b), 1981, **103**, No.2, p.581-587.

46. Shluger A.L., Kotomin E.A. Semiempirical Calculations of Defect Properties in LiF Crystal. (I). Perfect crystal. -Phys. Stat. Solidi (b), 1981, **108**, No.2, p.673-681.

47. Kuzovkov V.N., Kotomin E.A. Kinetics of Diffusion-Controlled Defect Accumulation Restricted by Their Recombination. Sol.St.Comm., 1981, **40**, No.1, p.173-176.

48. Kotomin E.A., Shluger A.L. Quantum-chemical simulation of Frenkel pairs separation in a LiF crystal. Sol.St.Comm., 1981, **40**, p.669-672.

49. Kuzovkov V.N., Kotomin E.A. Kinetics of diffusion-controlled defect accumulation restricted by their recombination. -Sol.St.Comm., 1981, **40**, p.173-176.

50. Tiliks Yu., Dzelme Yu., Kotomin E.A., Shluger A.L. Quantum chemical studies of the Electronic Structure, Mechanisms of Radiation Defect Creation and Recombination in Alkali Halide Crystals. Riga, 1981, Preprint No.30, 11p.

51. Kotomin E.A., Nagornyi A.N., Tale I.A., Tale V.G. Impurity hopping recombination in mixed and heavily-doped alkali halide crystals. -In: Int.Conf. on Defects in Insulating Materials. Riga, 1981, Preprint No.26.

1982

52. Kotomin E.A., Shluger A.L. Semiempirical Calculations of Defect Properties in LiF Crystal. (II). Electronic and Hole Centres and Their Recombination. -Phys. Stat. Solidi (b), 1982, **109**, No.1, p.75-81.

53. Kuzovkov V.N., Kotomin E.A. Effects of reagent density fluctuations on bimolecular reaction kinetics. -Chem. Phys. Lett., 1982, **87**, No.6, p.575-578.

54. Shluger A.L., Kotomin E.A., Kantorovich L.N. Calculation of Energies of Radiative Tunnelling Transitions between Defects in Alkali Halides. -Sol.St.Comm., 1982, **42**, No.10, p.749-752.

55. Ermoshkin A.N., Kotomin E.A., Shluger A.L. The semiempirical approach to the electronic structure of ionic crystals. -J.Phys.C: Sol.St.Phys., 1982, **15**, p.847-861.

56. Kuzovkov V.N., Kotomin E.A. Rigorons treatment of the spatial correlation of defects in kinetics of their accumulation and annealing. -Proc.Latv.Aca.Sci., 1982, No.1, p.42-49.

57. Kuzovkov V.N., Kotomin E.A. A role of reactant spatial correlations in bimolecular reaction kinetics. -Sov. Khim. phys., 1982, **1**, No.7, p.972-975.

58. Kotomin E.A., Kuzovkov V.N. Two approaches in the theory of bimolecular reactions. -Sov. theor. exp. chem., 1982, **18**, No.3, p.274-279.

59. Kuzovkov V.N., Kotomin E.A. Occupation number approach in the theory of diffusion-controlled reactions. -Proc.Latv.Aca.Sci., 1982, No.6, p.117-120.

60. Kotomin E.A., Shluger A.L., Tale I.A., Kurman I.S. Quantum chemical simulation of Frenkel defect creation and tunnelling recombination in alkali halides. -Probl.atom.sci. and technol., Kharkov phys.-techn. Inst., 1982, v.2 (21), p.33-35.

61. Ermoshkin A.N. Kotomin E.A., Tale I.A., Evarestov R.A. The position of Tl impurity level with respect to the perfect crystal bands. -Sov.Opt. and Spectr., 1982, **53**, No.1, p.186-188.

1983

62. Kotomin E.A., Shluger A.L., Tale I.A. Electronic structure of thallous centres and $Tl^+ - V_k$ recombination in KCl crystal. -Sol. St. Comm., 1983, **46**, No. 8, p.625-629.

63. Kuzovkov V.N., Kotomin E.A. Some problems of the recombination kinetics. (I). -Chem.Phys., 1983, **76**, No.3, p.479-487.

64. Kotomin E.A., Kuzovkov V.N. Some problems of the recombination kinetics. (II). -Chem. Phys., 1983, **81**, No.3, p.335-347.

65. Shluger A.L., Kotomin E.A. Modified INDO method for calculating point defects in ionic crystals. -Sov. theor. exp. chem., 1983, **19**, No.4, p.393-400.

66. Kuzovkov V.N., Kotomin E.A. Spatial correlation of reactants during the $A+B \to B$ reaction. -Proc. Latv. Aca. Sci., 1983, No.1, p.43-49.

67. Kotomin E.A., Shluger A.L., Ermoshkin A.N. Semiempirical calculations of the ionic surfaces. -Sov. J. phys. chem., 1983, **57**, No.5, p.1181-1185.

68. Kotomin E.A., Kuzovkov V.N. Generalized kinetics of the accumulation and recombination of radiation defects in solids. Probl.atom.sci. and technol., Kharkov phys.-techn. Inst., 1983, v.1(24), p.27-29.

69. Shluger A.L., Kotomin E.A., Dzelme Yu.R. Semiempirical calculations of the electronic structure of quasi-molecular centres in LiF crystal. -Probl.atom.sci. and technol., Kharkov phys.-techn. Inst., 1983, v.1(24), p.30-33.

1984

70. Kotomin E.A., Kuzovkov V.N., Tale I.A. Accumulation kinetics of immobile Frenkel defects incorporating their aggregation. -Proc. Latv. Aca. Sci., 1984, No.4, p.114-116.

71. Kuzovkov V.N., Kotomin E.A. Many-particle effects in Frenkel defect accumulation kinetics in crystals. -J.Phys.C: Sol.St.Phys., 1984, **17**, No.13, p.2283-2292.

72. Kotomin E.A. Temperature and impurity concentration dependence of the efficiency of Frenkel defect accumulation in alkali halide crystals. -Sol. St. Comm., 1984, **51**, No.4, p.225-229.

73. Kotomin E.A. Effective radius of diffusion-controlled tunnelling recombination incorporating Coulomb interaction. -Sov. Khim. phys., 1984, **3**, No.4, p.581-584.

1985

74. Kuzovkov V.N., Kotomin E.A. Some problems of the recombination kinetics. (III). -Chem. Phys., 1985, **98**, No.3, p.357-360.

75. Kotomin E.A., Kuzovkov V.N. Many-particle effects in kinetics of bimolecular diffusion-controlled reactions. -Chem. Phys. Lett., 1985, **117**, No.3, p.266-270.

76. Kuzovkov V.N., Kotomin E.A. Peculiarities of the diffusion- controlled recombination kinetics at long time and/or great reactant concentrations. -Czech. J. Phys., 1985, **B35**, p.541-548.

77. Kotomin E.A. Annealing kinetics of spatially correlated Frenkel defects in crystals. -Proc. Latv. Aca. Sci., 1985, No.5, p.122-124.

78. Kantorovich L.N., Kotomin E.A., Shluger A.L. Quantum chemical simulations of both electronic and spatial structure of defects in wide-gap solids. -Electr. processes and defects in ionic solids. Riga: Latv.Univ.press, 1985, p.146-166.

79. Shluger A.L., Kotomin E.A., Zakis Yu.R. Relation between properties of crystalline and glassy silicon dioxide and neutral interacting SiO_2 molecules. -Probl. of the glassy state physics. Riga: Latv.Univ.press, 1985, p.124-141.

80. Shluger A.L., Kantorovich L.N., Kotomin E.A., Dzelme Yu.R. Influence of alkali halide crystal surface upon the electronic structure of defects and their interaction with adsorbed water. -Sov.phys.chem., 1985, **59**, No.5, p.1224-1228.

81. Shluger A.L., Zakis Yu.R., Kotomin E.A. Relation between the electronic density distribution and the structural elements of solids. -Proc. Latv. Aca. Sci., 1985, No.12, p.73-100.

1986

82. Belevich I.V., Kotomin E.A., Shluger A.L., Evarestov R.A. The electronic structure calculations of thallium chlorides. -Proc. Latv. Aca. Sci., 1986, No.6, p.54-60.

83. Evarestov R.A., Belevich I.V., Kotomin E.A., Shluger A.L. The TlCl crystal electronic structure. -Sov.phys. -Solid State, 1986, **28**, No.4, p.1254-1256.

84. Shluger A.L., Kotomin E.A. Kantorovich L.N. Quantum-chemical simulation of impurity - induced trapping of a hole:$[Li]^0$ centre in MgO. -J. Phys. C: Sol.St.Phys., 1986, **19**, p.4183-4199.

1987

85. Causá M., Dovesi R., Kotomin E., Pisani C. MgO (110) surface and CO adsorption thereupon: *ab initio* study. (I). Clean (110) surface. -J.Phys.C: Sol.St.Phys., 1987, **20**, p.4383-4390.

86. Causá M., Kotomin E., Pisani C., Roetti C. MgO (110) surface and CO adsorption thereupon: *ab initio* study. (II). CO adsorption. -J.Phys.C: Sol.St.Phys., 1987, **20**, p.4391-4398.

87. Causá M., Dovesi R., Roetti C., Kotomin E., Saunders V.R. *ab initio* Hartree-Fock calculations of corundum.- Chem. Phys. Lett., 1987, **140**, No.2, p.120-123.

88. Kotomin E.A., Shluger A.L. Quantum chemical analysis of processes of defect creation in non-metallic crystals. -Sov. J. phys. chem., 1987, **61**, No.3, p.745-755.

1989

89. Kotomin E., Tale I., Tale V., Butlers P., Kulis P. Kinetics of non-steady state diffusion-controlled tunnelling recombination of defects in insulating crystals. -J.Phys.: Condens. Matter, 1989, **1**, No.38, p.6777-6784.

90. Kotomin E.A., Shluger A.L. Quantum-chemical simulation of defect creation in insulating crystals. -Radiation Effects and Defects in Solids, 1989, **111/112**, p.177-190.

91. Rogulis U., Kotomin E. Non-steady-state tunnelling recombination in insulating solids, controlled by defect diffusion and rotation. -Ibid.,1989, **111/112**, p.191-205.

92. Grigorjeva L.G., Millers D.K., Kotomin E.A. Short-lived radiation defects in silver halides. -Sov. Opt. Spectr., 1989, **67**, No.3, p.608-613.

1990

93. Artjushenko V., Antoniv I., Danev C., Kotomin E., et al. Formation and interaction of defects in silver halide crystals. - Infrared optics II: SPIE Proc., 1990, **1228**, No.13, p.140-150.

94. Kotomin E., Shluger A., Causá M., Dovesi R., Ricca F. The adsorption of SiO molecules on MgO surfaces as a model for the silicon lever atomic force microscope (AFM). - Surface Sci., 1990, **232**, No.3, p.399-406.

1991

95. Kotomin E. Computer simulations of hopping-controlled exchange reactions. -In: Dynamical processes in condensed molecular systems./ Eds. A.Blumen, J.Klafter, D.Haarer. (Singapore: World Scientific, 1991). P. 414-424.

96. Millers D.K., Grigorjeva L.G., Kotomin E.A., Krivads E., Eglitis R. High excitation density luminescence as a probe of mixed silver halides. - Proc. SPIE (Infrared Fiber Optics III). 1991, **15**, p.157-161.

1992

97. Kotomin E.A., Eglitis R.I., and Popov A.I. Kinetics of correlated annealing of radiation defects in ionic solids. -Nucl.Instr. & Meth. in Phys. Res.B, 1992, **65**, p.5l2-5l5.

98. Kotomin E.A., Popov A.I., Eglitis R.I. Correlated annealing of radiation defects in KBr crystals. -J.Phys.: Cond.Matt., 1992, **4**, p. 5901-59l0.

99. Grigorjeva L.G., Millers D.K., Kotomin E.A. Luminescence of mixed silver halide crystals under high excitation densities. -Sov. J. Appl. Spectr. 1992, **55**, No. 5, p.826-831.

100. Kotomin E.A., Kantorovich L.N., Tale I.A., Tale V., Phenomenological theory of V_k centre migration in KCl. -J.Phys.: Cond.Matt., 1992, **4**, p.7429-7440.

101. Jacobs P.W.M., Kotomin E.A., Stashans A., Tale I.A., Stefanovich E.V. Quantum-chemical simulations of hole self-trapping in corundum. - J.Phys.: Condens. Matter, 1992, **4**, p.7531-7544.

102. Kuzovkov V.N., Kotomin E.A. Self-organization in the $A + B \rightarrow 0$ reaction of charged particles. - Physica A, 1992, **191**, p.172-176.

103. Jacobs P.W.M., Kotomin E.A. Quantum Chemical Simulation of the Self-Trapped Hole in α-Al_2O_3 Crystals. - Phys. Rev. Lett., 1992, **69**, p.1411-1414.

1993

104. Millers D.K., Kotomin E.A., Grigorjeva L.G., Eglitis R.I. Short-lived luminescence of mixed silver halides. - J. Lumin., 1993, **55**, p.243-252.

105. Jacobs P.W.M., Kotomin E.A. Defects Energies for Corundum Doped with Transition Metal Ions. - Phil. Mag. A, 1993, **68**, p.695-709.

106. Jacobs P.W.M., Kotomin E.A., Stashans A., Tale I.A. Mechanism of Self-Trapped Hole Motion in Corundum Crystals. - Phil. Mag. B, 1993,**67**, p.557-567.

107. Jacobs P.W.M., Kotomin E.A. Theory of point defects and vacancy motion in corundum crystals. - J. Solid State Chem., 1993, **106**, p.27-34.

108. Millers D.K., Grigorjeva L.G., Kotomin E. Intrinsic luminescence of mixed silver halides under powerful excitation as a probe of solid solution composition. -In: Proc.Int. Conf. on Defects in Insulating Materials (World Scientific: Singapore, 1993) ,p.1277-1280.

109. Kotomin E.A., Kuzovkov V.N. Cooperative phenomena in bimolecular reactions in solids with point defects. - Ibid., p.1000-1003.

110. Jacobs P.W.M., Kotomin E.A. Calculations of oxygen vacancy hopping in $\alpha - Al_2O_3$ crystal. - Ibid., p.216-218.

111. Jacobs P.W.M., Kotomin E.A., Stashans A., Tale I., Stefanovich E. Computer simulations of hole self-trapping in $\alpha - Al_2O_3$ crystal. - Ibid., p.679-681.

112. Kotomin E.A., Eglitis R., Popov A.I. Kinetics of correlated difusion-controlled annealing of Frenkel defects in alkali halide crystals. - Ibid., p.1004-1006.

113. Kotomin E.A., Puchin V.E., Jacobs P.W.M. Theoretical simulation of H center migration in alkali halides: KCl and NaCl. - Phil.Mag.A, 1993, **68**, p.1359-1367.

114. Kuzovkov V.N., Kotomin E.A. Effect of non-equilibrium charge screening in the $A + B \to 0$ bimolecular reaction in condensed matter. - J. Stat. Phys., 1993, **72**, p.127-144.

115. Kuzovkov V.N., Kotomin E.A. The kinetics of defect accumulation under irradiation: many-particle effects. - Physica Scripta, 1993, **47**, p.585-595.

116. Popov A.I., Kotomin E.A., Eglitis R.I. The kinetics of correlated annealing of F, I centers in KBr crystals. - Phys. Stat. Solidi (b), 1993, **175**, K39-42.

117. Kotomin E., Zaiser M. A mesoscopic approach to point-defect clustering in solids during irradiation.- Appl. Phys. A, 1993, **57**, p.117-121.

118. Kuzovkov V.N., Kotomin E.A. Dynamical Particle Aggregation in the Bimolecular $A + B \to 0$ Reaction. - J.Chem.Phys., 1993, **98**, p.9107-9114.

119. Kotomin E.A., Zaiser M., Soppe W. A Mesoscopic Approach to Radiation-Induced Defect Aggregation in Alkali Halides Stimulated by Elastic Interaction of Mobile Frenkel Defects. - 1993, ECN Report RX-93-078.

1994

120. Jacobs P.W.M., Kotomin E.A., Stashans A., Tale I.A. Theoretical simulations of hole centers in corundum crystals. - Modelling and Simulations in Materials Science and Engineering, 1994, **2**, p.109-117.

121. Kotomin E., Kuzovkov V., Seeger A., Frank W. Reaction kinetics beyond rate equations: A correlation-function study of the effects of space dimension and reaction mobilities on the bimolecular annihilation reaction. - J.Phys. A: Math.& Gen. Phys., 1994, **27,** p.1453-1462.

122. P.W.M.Jacobs, E.A.Kotomin. Modelling of point defects in corundum crystals, J. Amer. Ceramic Soc., 1994, **77**, p.2505-2508.

123. Kotomin E.A., Zaiser M., Soppe W. A Mesoscopic Approach to Radiation-Induced Defect Aggregation in Alkali Halides Stimulated by Elastic Interaction of Mobile Frenkel Defects. - Phil. Mag. A, 1994, **70**, p. 313-327.

124. Soppe W., Kotomin E. Aggregation of Frenkel Defects Under Irradiation: A Mesoscopic Approach. - Nucl. Instr. Methods B, 1994, **91**, p.87-91.

125. Kantorovich L., Stashans A., Kotomin E., Jacobs P.W.M. Quantum Chemical Simulation of Hole Self-Trapping in Semi-Ionic Solids. - Int. J. Quant. Chem., 1994, **52**, p.1177-1198.

126. Kuzovkov V., Kotomin E. Pair and Triple Correlations in the $A+B \rightarrow B$ Diffusion-Controlled Reaction. - Phys. Rev. Lett, 1994, **72**, p.2105-2108.

127. Kotomin E.A., Jacobs P.W.M. Theoretical Simulations of Radiation- Induced Defect Processes in Insulating Materials. - Nucl. Instr. Methods B, 1994, **91**, p.52-59.

128. Kotomin E.A., Eglitis R.I., and Popov A.I. The kinetics of diffusion- controlled annealing of Frenkel defects in alkali halide crystals. - Nucl. Instr. Methods B, 1994, **91**, p.83-86.

129. Kotomin E.A., Millers D.K., Grigorjeva L.G., and Eglitis R.I. The Kinetics of Excitonic Luminescence in Mixed Silver Halides.- Proc. MRS Meeting, Symposium P, San Francisco (ed. M.J. Weber), 1994, **348**, p.309-312.

130. Kotomin E.A., Stashans A., and Popov A.I. A novel Model of $F^+ \rightarrow F$ Center Photoconversion in Corundum Crystals. - J.Phys: Condens. Matter, 1994, **6**, p.L569-L573.

131. Stashans A., Kotomin E.A., and Calais J.-L. Calculation of the ground and excited states of F-type centers in corundum crystals. - Phys. Rev .B, 1994, **49**, p.14854-14858.

132. Kuzovkov V.N. and Kotomin E.A. The Kinetics of F Center Aggregation Under Irradiation: Many-Particle Effects in Ionic Solids - Physica Scripta, 1994, **50**, p.720-725.

133. Kotomin E.A., Popov A.I., and Hirai M. The Recombination Kinetics of Frenkel Defects in Alkali Halides: Contradiction between Pulsed and Steady-State Studies. - J. Phys.Soc. Japan, 1994, **63**, p.2602-2611.

1995

134. Stashans A., Calais J.-L., and Kotomin E.A. Quantum Chemical Simulations of Point Defects in $\alpha - Al_2O_3$ Crystals. - Proc. 1.Eur. Conf. on Comput. Chemistry; Amer. Inst. of Phys., Proceedings **330**, (AIP Press, Woodbury, New York, 1995), p.176-182.

135. Popov A.I., Eglitis R.I. and Kotomin E.A. Theoretical Simulations of I-Center Annealing in KCl and KBr Crystals. - Rad.Eff.& Def.in Solids, 1995, **134**, p.83-86.

136. E.A.Kotomin, A.Stashans and P.W.M.Jacobs. Modelling of Point Defects in $\alpha - Al_2O_3$.- Ibid, p.87-90.

137. Kotomin E.A., Kuzovkov V.N., Zaiser M., and Soppe W. Theory of Diffusion-Controlled Defect Aggregation Under Irradiation: A Comparative Study of Three Basic Approaches. - Ibid, **136**, p.209-215

138. Grigorjeva L.G., Millers D.K., Kotomin E.A., and Eglitis R.I. The Kinetics of Excitonic Decay in AgCl Crystals. - J.Phys: Condens. Matter, 1995, **7**, p.1483-1491.

139. Eglitis R.I, Popov A.I., and Kotomin E.A. Computer Simulations of I-Center Annealing in KCl and KBr Crystals.- Phys. Stat. Solidi B, 1995, **190**, p.353-362.

140. E.A.Kotomin, A.Stashans, L.N.Kantorovich, A.I.Livshits, A.I.Popov, I.A.Tale, J.-L.Calais. Calculations of the geometry and optical properties of F_{Mg} centers and dimer (F_2-type) centers in corundum crystals. - Phys. Rev B, 1995, **51**, p.8770-82.

141. Jacobs P.W.M., Rycerz Z.A., and Kotomin E.A. Computer Simulation of Frenkel Defects in MgO and Li_2O. - Ukrainian J.Phys., 1995, **40**, p. 683-692. [Proc.Int.Pekar Conf., Odessa, October, 1994].

142. Kuzovkov V.N. and Kotomin E.A. The kinetics of colloid formation in solids under irradiation.- J.Phys.: Condens. Matter, 1995, **7**, L481-486.

143. Kuklja M.M., Kotomin E.A. and Popov A.I. Theoretical simulations of the electron center diffusion in MgO crystals. - Latvian Journal of Physics and Technical Sciences, 1995, No 5, p. 28-36.

1996

144. Svane A., Kotomin E.A., and Christensen N.E. First Principles Calculations of the vibrational properties of H centers in KCl Crystals.- Phys. Rev. B, 1996, **53**, p. 24-27.

145. Brudevoll T., Kotomin E.A., and Christensen N.E. Mechanism of interstitial oxygen atom diffusion in MgO.- Phys. Rev.B, 1996, **53**, p. 7731-7735.

146. Kotomin E.A., Grigorjeva L.G., and Miller D.K. The decay kinetics of diffusion-controlled excitonic luminescence in $AgCl_xBr_{1-x}$ solid solutions. - Proc. Int. Conf. on Excitonic Processes in Condensed Matter, (Dresden University Press, ed. M. Schreiber, 1996), p. 303-307.

147. Heifets E., Kotomin E.A., and Orlando R. Hartree-Fock simulation of Ag/MgO interface structure. - J. Physics: Condens. Matter, 1996, **8** , p. 6577 - 6584.

148. Eglitis R.I., Kuklja M.M., Kotomin E.A., Stashans A., and Popov A.I. Semi- empirical simulations of the electron centers in MgO. - Comp. Mater. Sci., 1996, **5**, p. 298-306.

149. Kuzovkov V.N., Kotomin E.A., and von Niessen W. Effect of reactant spatial distribution in the $A + B \to 0$ reaction kinetics in one dimension with Coulomb interaction. - Phys. Rev. E , 1996, **54**, p. 6128-6138.

150. Popov A.I., Kotomin E.A., and Kuklja M.M. Quantum Chemical Calculations of the Electron Center Diffusion in MgO. - Phys. Stat. Solidi B, 1996, **195**, p.61-66.

151. Kotomin E.A. and Kuzovkov V.N. Microscopic theory of colloid formation in solids under irradiation.- Mater. Sci & Eng. B, 1996, **37**, p. 49-51.

152. Kotomin E.A., Kuklja M.M., Eglitis R.I., and Popov A.I. Quantum Chemical Simulations of the Optical Properties and Diffusion of Electron Centers in MgO Crystals. - Ibid., p. 212-214.

153. Grigorjeva L.G., Millers D.K., Kotomin E.A., Eglitis R.I, and Lerman A.A. Optical Properties of Silver Halide Fibers: Extrusion and Aging Effects. - J. Phys.D: Applied Physics, 1996, **29**, p. 578-583.

154. Kotomin E.A., Svane A., Brudevoll T., Schulz W., and Christensen N.E. First-Principles Simulations of Interstitial Atoms in Ionic Solids. - Proc. Fall MRS Meeting, Boston, Symp. P.(Materials Theory, Simulations and Parallel Algorithms), 1996, **408**, p. 509-512.

155. Kuzovkov V.N., Kotomin E.A., and W. von Niessen. The kinetics of the bimolecular $A + B \to 0$ reaction in condensed matter: effects of non-equilibrium charge screening. - J. Chem. Phys., 1996, **105**, p.9486-9492.

156. Kalnin Yu.R.H and Kotomin E.A. Many-particle peculiarities in the $A + B \to B$ bimolecular reaction kinetics. The effect of sink spatial distribution. - J. Phys.: Condens. Matter, 1996, **8**, 6729- 6735.

157. Kalnin Yu.H. and Kotomin E.A. A comparison of the effective medium and modified Smoluchowski equations for the reaction rate of diffusion-controlled reactions. - J. Nuclear Mater., 1996, **232**, 253-255.

158. Heifets E. and Kotomin E.A. The electronic and atomic structure of Ag/MgO interface. -Latvian Journal of Physics and Technical Sciences, No **5**, 53-70 (1996).

1997

159. Puchin V.E., Shluger A.L., Gale J.P., Kotomin E.A., Günster J., Brause M. and Kempter V. Atomic structure of the (0001) corundum surface. - Surf. Sci., 1997, **370**, p. 190-200.

160. Zhukovskii Yu.F., Kotomin E.A., Nieminen R., and Stashans A. Quantum chemical simulations of free and bound hole polarons in corundum crystals. - Comput. Mater. Sci., 1997, **7**, p. 285-294.

161. Puchina A.V., Puchin V.E., Kotomin E.A., and Reichling M. *Ab initio* study of the F center in CaF_2 crystal. - Preprint Int. Center for Theor. Phys., IC/97/112.

162. Jacobs P.W.M., Kotomin E.A., Christensen N.E. and Brudevoll T. Theory of diffusion and aggregation of radiation-induced defects in MgO and $\alpha - Al_2O_3$ crystals. - Materials Science Forum (Trans Tech Publications Ltd., Switzerland, 1997), Proc. Int. Conf. on Defects in Insulating Materials (ICDIM-96), p. 391-394.

163. Kotomin E.A. and Kuzovkov V.N. The kinetics of radiation-induced defect accumulation in ionic solids. - Ibid., p. 387-391.

164. Puchin V.E., Gale J.P., Shluger A.L., Kotomin E.A., Günster J., Brause M. and Kempter V. Atomic structure of the (0001) corundum surface. - Ibid., p. 633-636.

165. Zhukovskii Yu.F., Kotomin E.A., Nieminen R., Devreese J.T., and Stashans A. Quantum chemical simulations of bound hole polarons (V_{Mg} centers) in corundum crystals.- Proc. SPIE (Int. Conf. on Advanced Optical Materials and Devices, AOMD-96, Riga, August 1996), vol **2967** , p. 153-158.

166. Eglitis R.I. and Kotomin E.A. Calculations of F centers in $KNbO_3$, Ibid., p.150-152.

167. Jacobs P.W.M., Kotomin E.A., and Evarestov R.A. Formation, diffusion and aggregation of radiation- induced defects in MgO and $\alpha - Al_2O_3$ crystals. - Ibid., p. 132-137.

168. Kotomin E.A. Semi-empirical simulations of radiation defects in oxide materials. - Computer Modelling of Electronic and Atomic Processes in Solids ed. R.C.Tennyson and A.E.Kiv (Proc. NATO workshop on the Electronic and Space Materials Wroclaw, Poland, May 1996), NATO ASI series , (Kluwer Academic Publishers, Dordrecht/Boston/London, 1997) p.51-59.

169. Heifets E., Dorfman S., Fuks D., and Kotomin E.A. Atomistic Simulations of the (001) surface structure for $BaTiO_3$. - Thin Solid Films, 1997, **296**, p.76-78.

170. Kuklja M.M., Kotomin E.A., Popov A.I. Semi-empirical simulations of F-center diffusion in KCl crystals.- J. Phys. Chem. Solids, 1997, **58**, p. 103-106.

171. Kuzovkov V.N. and Kotomin E.A. Theory of diffusion-controlled colloid formation in irradiated solids. - Solid State Ionics, 1997 (Proc. Int. Conf. on Reactivity of Solids, Hamburg, 1996), **101-103**, p.451-455.

172. Kotomin E.A., Jacobs P.W.M., Christensen N.E., Brudevoll T., Kuklja M.M., and Popov A.I. Calculations of diffusion and aggregation energies for intrinsic defects in MgO . - Defects and Difusion Data (Proc. Int. Conf. on Diffusion in Materials, DIMAT-96, Nordkirchen, 1996), 1997, pt. A, **143-147**, p.1231-36.

173. Zhukovskii Yu.F., Sokol A., Kotomin E.A., Catlow C.R.A., and Nieminen R. Semiempirical supercell calculations of bound hole polarons (V_{Mg} centers) in $\alpha - Al_2O_3$ crystals. - J. Phys.: Condens. Matter, 1997, **9**, 3559-73.

174. Eglitis R.I, Christensen N.E., Kotomin E.A., Postnikov A., and Borstel G. First principles and semi-empirical calculations for F centers in $KNbO_3$. - Phys. Rev. B, 1997, **56**, p. 8599-8604.

175. Kotomin E.A., Eglitis R.I., and Popov A.I. Charge distribution and optical properties of F^+ and F centers in $KNbO_3$ crystal. - J.Phys.: Condensed Matter, 1997, **9**, L315-321.

176. Grigorjeva L., Millers D.K., Popov A.I., Kotomin E.A. and Polzik E.S. Luminescence Properties of $KNbO_3$ crystals. - J. Lumin., 1997, **72-74**, (Proc. Int. Conf. on Lumin., Prague, August 1996), p. 672-674.

177. Kalnin Yu.R., Zvejnieks G. and Kotomin E.A. The diffusion-controlled energy transfer rate for a paired sink distribution. - Phys. Status Solidi B, 1997, **201,** p. 339-342.

178. Grigorjeva L., Millers D., Kotomin E.A., and Polzik E.S. Transient optical absorption in $KNbO_3$crystals irradiated with pulsed electron beam. -Solid State Comm., 1997, **104**, p. 327-330.

179. Dorfman S., Heifets E., Fuks D., Kotomin E.A., and Felsteiner J. Surface relaxation in ferroelectric perovskites: an atomistic study. - Proc. MRS meeting (Boston, December 1996) *Materials for Smart Systems II*, 1997, v. **459**, p.219-225.

180. Puchin V.E., Kotomin E.A., and Shluger A.L. Atomic structure of the (0001) corundum surface. Proc. MRS meeting (Boston, December 1996), 1997, v. **453**, p. 721-726.

181. Kotomin E.A. and Kuzovkov V.N. Theory of Diffusion-Controlled Colloid Formation in Irradiated Solids. - -Latvian Journal of Physics and Technical Sciences, 1997, No 1, p. 3-15.

182. Kalnin Yu.R.H., Zvejnieks G., and Kotomin E.A. The effect of particle generation function on the rate of diffusion-controlled $A + B \to B$ reaction with a permanent particle source.- Chem. Phys. Lett., 1997, **270**, p. 229-233.

183. Kotomin E.A., Kuzovkov V.N., and von Niessen W. Pattern formation and unusual $A + B \to 0$ reaction kinetics between charged reactants in low dimensions. - Proc. MRS, 1997, **463** (Statistical Mechanics and Physics and Biology), p. 275-280.

1998

184. Kotomin E.A. and Kuzovkov V.N. Microscopic theory of diffusion-controlled defect aggregation. – Comput. Mater. Sci., 1998, **10**, p. 22-27.

185. Kotomin E.A., Christensen N.E., Eglitis R.I., and Borstel G. A comparative study of the electronic and atomic structure of F centers in ferroelectric $KNbO_3$: ab initio and semi-empirical calculations. – Comput. Mater. Sci. 1998, **10**, p.339-345.

186. Fuks D., Dorfman S., Heifets E., Kotomin E., and Gordon A. Atomistic study of surface polarisation in superconducting perovskites. - In: "Structure and Evolution of Surfaces", Proc. MRS, 1998, **440**,p. 305-310.

187. Dorfman S., Fuks D., and Kotomin E.A. Comparative study of (001) surface relaxation for some titanates. - Thin Solid Films, 1998, **318**, p. 65-68.

188. Zhukovskii Yu.F., Heifets E., Kotomin E.A., and Nieminen R.M. *Ab initio* study of the electronic and atomic structure of the Ag/MgO interface.-.Proc. 7 Europ. Conf. on Applications of Surfaces and Interface Analysis (ECASIA-97, Göteborg, June 1997), p. 117-120.

189. Zhukovskii Yu.F., Alfredsson M., Hermansson K., Kotomin E.A., and Nieminen R.M. Ab simulations of CO adsorption on both clean and Ag-predosed (0001) corundum surfaces. - Ibid., p.197-200.

190. Kotomin E.A., Popov A.I., and Stashans A. Computer Modelling of Radiation Damage in Cation Sublattice of Corundum. - Phys. Stat. Solidi, 1998, **B 207**, p. 69-73.

191. Kotomin E.A. and Popov A.I. Radiation-Induced Point Defects in Simple Oxides. - Proc. Int. Conference on Radiation Effects in Insulators (REI-9), Nuclear Instruments and Methods, 1998, **B 141**, p.1-15.

192. Huisinga M., Bouchaala N., Bennewitz R., Reihling M., Kotomin E.A., Matthias E., Kuzovkov V.N., and von Niessen W. The kinetics of CaF_2 Metalization Induced by Low-Energy Electron Irradiation. - Ibid., p. 79-84.

193. Zhukovskii Yu.F., Alfredsson M., Hermansson K., Heifets E., and Kotomin E.A. *Ab initio* simulations of silver film adhesion on A_2O_3 (0001) and MgO (001) surfaces. - Ibid., p. 73-78.

194. A.V.Puchina, V.E. Puchin, E.A. Kotomin, and M.Reichling, *Ab initio* study of F centers in CaF_2 crystals. - Solid State Comm., 1998, **106**, p. 285-288.

195. Kuzovkov V.N., Kotomin E.A.and W. von Niessen. The discrete-lattice theory of colloid formation in irradiated solids. - Phys. Rev. B, 1998, **58**, p.8454-63.

196. Heifets E., Dorfman S., Fuks D., Kotomin E.A., and Gordon A. Atomistic simulation of $SrTiO_3$ (001) surface relaxation. - J. Phys.:Cond. Matter, 1998, **10**, L 347-353.

197. Heifets E., Zhukovskii Yu., Kotomin E.A., and Causa M. The adhesion nature of Ag/MgO (100) interface: an *ab initio* study. - Chem. Phys. Lett., 1998, **283**, p. 395-401.

198. Popov A.I. and Kotomin E.A. A simple analysis of the H_A centre destruction temperature for doped alkali halides. - Solid State Comm., 1998, **106**, p. 289- 291.

199. Heifets E., Dorfman S., Fuks D., Kotomin E.A., and Gordon A. (001) surface structure in $SrTiO_3$. Atomistic study. - Surface Reviews and Letters, 1998, **5**, p. 341-346.

200. Kalnin Yu.R. and Kotomin E.A. Modified Maxwell-Garnett equation for the effective transport coefficients in inhomogeneous media.-J. Phys.A: General/ Math., 1998, **31**, p.7227-34.

201. Eglitis R.I., Kotomin E.A., and Borstel G. Semi-empirical Calculations of Hole Polarons in MgO and $KNbO_3$ Crystals. - Phys. Status Solidi, 1998, **B 208**, p. 15-20.

202. Dorfman S., Fuks D., Gordon A., Kotomin E.A., and Wyder P. Magnetic field tuning of the smart material domain structure. - Proc. SPIE, 1998, **3324**, p.276-286.

203. Eglitis R.I., Kotomin E.A., Postnikov A.V., Christensen N.E., and Borstel G. First-principles and semi-empirical calculations for the F centers in $KNbO_3$ and Li impurity in $KTaO_3$. In: First Principles Calculations for Ferroelectrics (5th Williamsburg Int. Workshop, ed. R.Cohen, Woodbury, N.Y., AIP Conference Proceedings **436**, p. 207-216, 1998).

204. Eglitis R.I., Kotomin E.A., Borstel G., and Dorfman S. Semi-empirical calculations of Nb ion positions in doped $KTaO_3$ crystals. - J. Phys.:Cond. Matt., 1998, **10**, p. 6271-76.

205. Eglitis R.I., Kotomin E.A., and Borstel G. Quantum Chemical Calculations of KTN Solid Solutions. – Solid State Comm., 1998, **108**, p. 333-336.

206. Bouchaala N., Kotomin E.A., Kuzovkov V.N., Reichling M. F center aggregation kinetics in low-energy electron irradiated LiF. - Solid State Comm., 1998, **108**, p.629-633.

1999

207. Millers D.K., Grigorjeva L., Kotomin E.A. Primary Radiation Defect Creation and Separation in AgBr. - Proc. Int. Conf. on Defects in Ionic Solids (Keele, July 1998), Radiation Effects and Defects in Solids, 1999, **150**, p.185-191.

208. Jacobs P.W.M., Kotomin E.A., Eglitis R.I. Semi-empirical INDO and shell-model calculations for perovskites. - Radiation Effects and Defects in Solids, 1999, **151**, p.243-247.

209. Yohum H.M., Ucer K.B., Williams R.T., Sheldon P.A., Nagirnyi A., Denks V., Grigorjeva L., Millers D.K., Kotomin E.A. Short- pulse excitation and spectroscopy of $KNbO_3$, $LiNbO_3$ and $KTiPO_4$. - Radiation Effects and Defects in Solids, 1999, **150**, p.271-276.

210. Monge M.A., Gonzalez R., Munoz-Santiuse J.E., Pareja R., Chen Y., Kotomin E.A., Popov A. Photoconversion and Dynamic Hole Recycling in Anion Vacancies in Neutron-Irradiated MgO Crystals. - Phys. Rev. B, 1999, **60**, p. 3787–3791.

211. Kuklja M.M., Stefanovich E.V., Kotomin E.A., Popov A.I. Gonzalez R., Chen Y. *Ab initio* and semi-empirical simulations of H^- centers in MgO crystals. - Phys. Rev. B, 1999, **59**, p.1885–1890.

212. Gonzalez R., Monge M.A., Munoz-Santiuse J.E., Pareja R., Chen Y., Kotomin E.A., Kuklja M.M., Popov A.I. Photoconversion of F-type centers in thermochemically reduced MgO single crystals. - Phys. Rev. B, 1999, **59**, p. 4786-4790.

213. Eglitis R.I., Kotomin E.A., Postnikov A.V., Christensen N.E., Borstel G., Philpott M.R. Computer simulations of defects in perovskites $KNbO_3$ crystals. – Ferroelectrics, 1999, **229**, p. 69-75. (Proc. 2nd Asian Meeting of Ferroelectrics, Singapore, 1998).

214. Kotomin E.A., Eglitis R.I, Postnikov A.I., Borstel G., Christensen N.E. First-principles and semi-empirical calculations for bound hole polarons in $KNbO_3$. - Phys. Rev. B, 1999, **60**, p. 1-5.

215. Monge M.A., Gonzalez R., Popov A.I., Pareja R., Chen Y., Kotomin E.A., Kuklja M.M. The dynamics of the hydrade ion in MgO crystals. - In: *Defect and Diffusion Forum*, 1999, **169/170**, p. 1-11.

216. Zhukovskii Yu.F., Kotomin E.A., Jacobs P.W.M., Stoneham A.M., Harding J.H. A comparative study of the Ag/MgO (100) and (110) interfaces. - Surf. Sci., 1999, **441**, p. 373–383.

217. Heifets E., Kotomin E.A., and Borstel G. Atomistic Simulations of the (110) Surface Relaxation for Perovskite Titanates. - Surf. Reviews and Letters, 1999, **6**, p.1215-1219. (Proc. ICSOS-6, Vancouver, July 1999), p.1215-1219.

2000

218. Jacobs P.W.M., Kotomin E.A., Eglitis R.I. Semi-empirical defect calculations for the perovskite $KNbO_3$. - J. Phys.: Cond. Matt., 2000, **12**, p.569-574.

219. Kotomin E.A., Heifets E., Jacobs P.W.M., Borstel G., Goddard W.A. Theoretical simulations of surface relaxation for perovskite titanates. - In: *Proc. NATO ARW on Defects and Surface- Induced Effects in Advanced Perovskites*, Riga, August 1999 (Kluwer 2000), p. 209-220.

220. Christensen N.E., Kotomin E.A., Eglitis R.I., Postnikov A.V., Novikov D.L., Tinte S., Stachiotti M.G., Rodriguez C.O. Theoretical modelling of $KNbO_3$ perovskites without and with defects. - Ibid., p. 3-16.

221. Kotomin E.A., Eglitis R.I., Borstel G. Quantum chemical modelling of point defects in $KNbO_3$ perovskite crystals. - (Proc. EuroMRS Meeting, Symposium C), Comput. Mater. Sci., 2000, **17** p. 290-298.

222. Zhukovskii Yu., Kotomin E.A., Jacobs P.W.M., Stoneham A.M., Harding J.H., Modelling of silver adhesion on MgO (100) surface with defects. - J. Phys.: Cond. Matter, 2000, **12**, p.55-66.

223. Kotomin E.A., Eglitis R.I., Borstel G., Grigorjeva L.G., Millers D.K., Pankratov V. - Theoretical and Experimental Study of Radiation Defects in $KNbO_3$ Perovskite Crystals. - Proc. Int. Conference on Radiation Effects in Insulators (REI-10). Nucl. Instr. Meth., 2000, **B166-167** , p. 299-304.

224. Monge M.A., Gonzalez R., Munos Santiuste J.E., Pareja R., Chen Y., Kotomin E.A., Popov A.I., Photoconversion of F^+ Centers in Neutron- Irradiated MgO. - Ibid., p. 220-224.

225. Kotomin E.A., Heifets E. Atomistic Simulation of $SrTiO_3$ and $BaTiO_3$ (110) Surface Relaxations. - Thin Solid Films, 2000, **358** , p.1-5.

226. Zhukovskii Yu., Kotomin E.A., Jacobs P.W.M., Stoneham A.M., Ab initio modelling of metal adhesion on oxide surfaces with defects. - Phys. Rev.. Lett., 2000, **84**, p.1256-1260.

226. Fuks D, Dorfman S., Zhukovskii Yu, Kotomin E.A., Stoneham A.M. Theoretical Analysis of the Growth Mode for the Metallic Films on Oxide Substrates. - Phys. Rev. Lett., 2000, **85**, p.4333-4336.

227. Monge M.A., Popov A.I., Ballesteros C, Gonzalez R., , Chen Y., Kotomin E.A. Formation of Anion Vacancy Clusters and Nano Cavities in Thermochemically Reduced MgO Single Crystals. – Phys. Rev. B, 2000, **62**, p. 9299-9304.

228. Heifets E., Kotomin E.A., Jacobs P.W.M. Calculations of the Atomic Structure of $KNbO_3$ (110) Surface.- Thin Solid Films, 2000, **374**, p.64-69.

229. Heifets E., Kotomin E.A., Maier J. Semi-empirical Simulations of Surface Relaxation for Perovskite Titanates.- Surface Science 2000, **462**, p.19-36.

230. Eglitis R.I., Kotomin E.A., Borstel G. Quantum Chemical Modelling of Perovskite Solid Solutions. - J. Phys.:Cond. Matt., 2000, **12**, p.L431-434.

231. Borstel G., Kotomin E.A., Eglitis R.I., Heifets E. Computer Modelling of Point Defects, Impurity Self-Ordering effects and Surfaces in Advanced Perovskite Ferroelectrics. - Acta Physica Polonica, 2000, **98**, p.469-481.

232. Kotomin E.A., Eglitis R.I., and Borstel G. Quantum chemical modelling of electron polarons and excitons in ABO_3 perovskites. - J. Phys.:Cond. Matt., 2000, **12**, p.L557-562.

233. Borstel G., Kotomin E.A., Eglitis R.I., Heifets E. Computer Modelling of Defects and Surfaces in Advanced Perovskites. – Jap. Journal of Applied Phys., 2000, **39**, suppl. 39-1, p.24-28.

2001

234. Eglitis R.I., Kotomin E.A., Borstel G. Quantum Chemical Modelling of Polarons and Perovskite Solid Solutions. – Comput. Mater. Science, 2001, **21**, p. 530-534.

235. Kalnin J.R., Kotomin E.A., Kuzovkov V.N. Calculation of the Effective Diffusion Coefficient in Inhomogeneous Solids. - Defect and Diffusion Forum, 2001, **194-1**, p. 163-167 (Proc. V Int. Conf. on Diffusion in Materials, Paris, July 2000).

236. Borstel G., Eglitis R.I., Kotomin E.A. Computer modeling of KTN solid solutions. - Proc. 12th Intern. Symp. on Applications of Ferroelectrics (ISAF, Hawaii), (S.K. Streiffer, B.J. Gibbson, and T. Tsurami, eds., Proc. IEEE, cat. No 00CH37076) 2001, vol.**2**, p. 671-674.

237. Zhukovskii Yu., Kotomin E.A., Fuks D., Dorfman S., Gordon A. Hartree–Fock study of adhesion and charge distribution on the Ag/MgO (001) interface. (Proc. Int. Conf. ICSOS-9, Madrid, July 2000) - Surf. Sci, 2001, **482-485**, p. 66-72.

238. Vikhnin V.S., Eglitis R.I., Kotomin E.A., Kapphan S.E., Borstel G. New Polaronic-Type Excitons in Ferroelectric Oxides. - Proc. Williamsburg Meeting on Fundamental Physics of Ferroelectrics, H. Krakauer (ed.), AIP Conference Proc.,N.Y., 2001, **vol. 582**, p.228-239.

239. Heifets E., Eglitis R.I., Kotomin E.A., Borstel G. First-principles and semi-empirical calculations of atomic and electronic structure for the (100) and (111) Perovskite Surfaces. – Ibid., p. 201-210.

240. Heifets E.I., Kotomin E.A., Eglitis R.I., Cohen R.E. Calculations of perovskite surface relaxation. – Proc. Fall-2000 Meeting of Materials Research Society. C.B. Carter, X. Pan, K. Sickafus, H.L. Tuller (eds.), Symp. AA, 2001, p. AA 5.3.1-6 (Boston 2001).

241. Devreese J.T., Fomin V.M., Pokatilov E.P., Kotomin E.A., Eglitis R.I, and Yu. F. Zhukovskii. - Phys. Rev., 2001, **B 63**, p. 184304-1-6.

242. Popov A.I., Monge M.A., Gonzalez R., Chen Y., and Kotomin E.A. - Dynamics of F-center annihilation in thermochemically reduced MgO single crystals. – Solid State Comm., 2001, **118**, p. 163-167.

243. Kuzovkov V.N., Popov A.I., Kotomin E.A., Monge M.A., Gonzalez R., and Chen Y. Kinetics of nanocavity formation based on F-center aggregation in thermochemically reduced MgO single crystals. – Phys. Rev., 2001, **64**, 064102, (p.1-5).

244. Kotomin E.A., Kashcheyevs V., Kuzovkov V.N., Schwartz K., and Trautmann C. Modelling of primary defect aggregation in tracks of swift heavy ions in LiF. - Phys. Rev. B, 2001, **64**, p. 144108 (1-7).

245. Heifets E., Eglitis R.I., Kotomin E.A., Maier J., and Borstel G. *Ab initio* modelling of surface structure for $SrTiO_3$ perovskite crystals. - Phys. Rev. B, 2001, **64**, p. 235417 (p.1-5).

246. Heifets E., Kotomin E.A., Eglitis R.I., and R.E. Cohen. Calculation perovskite surface relaxation. - Mat. Res. Soc. Symp. Proc., 2001, vol. **654** , p. AA5.3.1-6.(MRS Spring-2001 Meeting, San Francisco, April 2001)

247. Eglitis R.I., Kotomin E.A., and Borstel G. Computer modelling of luminescence in ABO_3 perovskites. - Mat. Res. Soc. Symp. Proc., 2001, vol.**667**, p.G.1.8.1-6.

248. Vikhnin V.S., Eglitis R.I., Kotomin E.A., Kapphan S.E., and Borstel G. New polaronic-type excitons in ferroelectric oxides: INDO calculations and experimental manifestation.- Mat. Res. Soc. Symp. Proc., 2001, vol. **677**, p. AA4.15.1-6.

249. Vikhnin V.S., Eglitis R.I., Kapphan S:E., Kotomin E.A., and Borstel G. A new phase in ferroelectric oxides: the phase of charge transfer vibronic exciton. - Europhys. Lett., 2001, **56**, p. 701-708.

250. Heifets E., Eglitis R.I., Kotomin E.A., and Borstel G. Calculations of surface structure for $SrTiO_3$ perovskite. – Mat. Res. Soc. Symp. Proc. 2001, vol. **672**, p. O9.1.1-6.

251. Yu. F. Zhukovskii, E.A. Kotomin, B. Herschend, K. Hermansson, and P.W.M. Jacobs. A first-principles study of the Ag/Al_2O_3 (0001) interface. - Int. J. of Molec. Sci., 2001, **2**, p. 271-280.

252. Dorfman S., Fuks D., Gordon A., Kotomin E.A., Wyder P. Some nonlinear properties of ferroelectric smart materials. – Physica B 2001, **304**, p. 339-347.

253. Kotomin E.A., Kuzovkov V.N., Popov A.N. The Kinetics of Defect Aggregation and Metal Colloid Formation in Insulating Solids under Irradiation. - Radiation Defects and Effects in Solids, 2001, **155**, p.113-125 (Proc. ICDIM-2000, Johannesburg)

254. Kashcheyevs V., Kotomin E.A., Kuzovkov V.N. Modelling of Metal Colloid Formation in Tracks of Swift Heavy Ions in Ionic Solids. - Ibid., p. 154-151.

255. E.A.Kotomin, R.I. Eglitis, J. Maier, and E. Heifets. Calculations of the atomic and electronic structure for $SrTiO_3$ perovskite thin films. - Thin Solid Films, 2001, **400** , p. 76-80 (Proc. EMRS, Symp. N, Strasburg, July 2001)

2002

256. Borstel G., Eglitis R.I., Kotomin E.A., and Heifets E. Modelling of defects and surfaces in perovskite ferroelectrics, J. of Crystal Growth, 2002, **237/239**, p. 687-693.

257. Kalnin J.R., Kotomin E.A., and Maier J. Calculations of the effective diffusion coefficient for inhomogeneous media. - J. of Phys. Chem. Solids, 2002, **63**, p. 449-454.

258. Fuks D., Dorfman S., Zhukovskii Yu., Kotomin E.A., and Stoneham A.M. Theory of the growth mode for a thin metallic film on an insulating substrate. - Surface Science, 2002, **499**, p. 24-40.

259. D. Fuks, S. Dorfman, Yu. Zhukovskii, E.A. Kotomin, A.M. Stoneham. Effect of electron correlation corrections on a phase competition in Ag film growth on MgO substrate. - Comput. Mater. Sci., 2002, **24**, p. 66-71. (Proc. EMRS, Symp. A, Strasburg, July 2001).

260. E.A. Kotomin and R.A. Evarestov. Large-scale *ab initio* modelling of defects in perovskites: Fe impurity in $SrTiO_3$. – Ibid., p. 14-20.

261. Yu. Zhukovskii, E.A. Kotomin, B. Herschend, K. Hermansson, and P.W.M. Jacobs. The adhesion properties of the Ag/corundum (0001) interface: an *ab initio* study. – Surf. Sci, 2002, **513**, p.343-358.

262. E.A. Kotomin, Yu. Zhukovskii, S. Dorfman, D. Fuks. Atomistic theory of the growth mode for a thin metallic film on an insulating substrate. – in: *Proc. NATO ARW on Atomistic Aspects of Epitaxial Growth, Corfu, June 2001*, (ed.M. Kotrla, N.Papanicolaou, D. Vvedensky, L.Wille, Kluwer 2002), p. 525-534.

263. Vikhnin V., Eglitis R., Kapphan S., Borstel G., Kotomin E.A. Polaronic-Type Excitons in Ferroelectric Oxides. – Phys. Rev. B, 2002, **65**, p. 104304, 1-11.

264. Kotomin E.A., Kuzovkov V.N., Popov A.I., Monge M.A., Gonzalez R., and Chen Y. Diffusion-controlled annihilation of F centers in thermochemically reduced MgO crystals. – Nucl. Instr. and Methods, 2002, **B 191**, (Proc. Radiation Effects in Insulators, REI-11, Lisbon, September 2001), p. 208-211.

265. Kotomin E.A., Maier J., Eglitis R., and Borstel G. Calculations of radiation- induced point defects, polarons and excitons in ferroelectric perovskites. – Ibid., p. 22-26.

266. Eglitis R., Kotomin E.A., Borstel G., and Vikhnin V.S. Computer modelling of point defects in perovskite crystals. – Ferroelectrics, 2002, **268**, p. 479-484.

267. Eglitis R., Heifets E., Kotomin E.A., and Borstel G. Calculations of Atomic and Electronic Structure for (100) Surfaces of $SrTiO_3$ Perovskite. – Mat. Res. Soc. Symp. Proc., 2002, vol. **718**, p. D10.16.1-6.(MRS Spring-2002 Meeting, San Francisco, April 1-5, 2002).

268. Eglitis R., Kotomin E.A., Christensen N.E., and Borstel G. Calculations of the Electronic and Atomic Structure and Diffusion of Point Defects in $KNbO_3$ Perovskite Crystals and Relevant KTN Solid Solutions. – Ibid, vol. **718**, p. D11.11.1-6

269. Evarestov R.A., Eglitis R., Piskunov S., Kotomin E.A., and Borstel G. Large scale *ab initio* Simulations of Fe-doped $SrTiO_3$. – Ibid., vol. **731**, p.W3.12.1-6.

270. Eglitis R., Vikhnin V.S., Kotomin E.A., Kapphan S.E., and Borstel G. Theoretical Prediction and Experimental Confirmation of Charge Transfer Vibronic Excitons and Their Phase in ABO_3 Perovskite Crystals. – Ibid., vol. **718**, p.D10.32.1-6.

271. Eglitis R., Kotomin E.A., Trepakov V.A., Kapphan S.E., and Borstel G. Quantum chemical modelling of electron polarons and green luminescence in $PbTiO_3$ perovskite crystals. – J. Phys.: Condens. Matter, 2002, **14**, p. L 647-L653.

272. Kotomin E.A., Maier J., Stoneham A.M., Zhukovskii Yu.F., Fuks D., and Dorfman S. *Ab initio* Modelling of Metal Adhesion to Ceramics. – Proc. CIMTEC–10 (International Ceramics Congress, Florence, July 15-18, 2002, Techna Publishers, ed. P. Vincentini), Part C, vol.3, p.669-682.

273. Fuks D., Dorfman S., Zhukovskii Yu.F., Kotomin E.A., and Stoneham A.M. Thermodynamics of the Initial Stage of Growth for a Thin Metallic Film on an Insulating Substrate. – Ibid., p. 683-694.

274. Eglitis R.I., Kotomin E.A., and Borstel G. Quantum chemical modelling of electron polarons and charge transfer vibronic excitons in $BaTiO_3$ perovskite crystals. – J. Phys.: Condens. Matter, 2002, **14**, p. 3735-3741.

275. Eglitis R.I., Kotomin E.A., and Borstel G. Quantum Chemical Modelling of Green Luminescence in ABO_3 Perovskites. – European J. of Physics B, 2002, **27**, p.483-486.

276. Heifets E., Eglitis R.I., Kotomin E.A., Maier J., and Borstel G. First-principles calculations for $SrTiO_3$ (100) surface structure. – Surf. Sci., 2002, **513**, p.211-220.

277. Heifets E., Eglitis R.I., Kotomin E.A. and Borstel G. *Ab initio* Calculations for $SrTiO_3$ (100) Surface Structure. – In: *Proc. Williamsburg Meeting on Fundametal Physics of Ferroelectrics– 2002*, R.E. Cohen and T. Egami (eds.), AIP Conf. Proc., **626**, N.Y., 2002, p.285-293.

278. Kashcheyevs V., Kotomin E.A., and Kuzovkov V.N. Modelling of primary defect aggregation in tracks of swift heavy ions in alkali halides. – Surface and Coating Technology, 2002, **C 158-159**, p. 269-272.

279. Kotomin E.A., Heifets E., Eglitis R.I., Maier J., and Borstel G. *Ab initio* modelling of the atomic and electronic structure of $SrTiO_3$ (100) surfaces. – Computer Modelling and New Technologies, 2002, **6**, N 2, p. 7-20.

2003

280. Zhukovskii Yu.F., Kotomin E.A., and Jacobs P.W.M. Large scale computer simulations of metal/oxide interfaces with defects. – Proc. SPIE, 2003 (Proc. Int. Conf. on Advanced Optical Materials and Devices, August 19-22, Riga), **5122**, p.104-111.

281. Borstel G., Eglitis R., and Kotomin E.A. Computer modelling of point defects, polarons and excitons in perovskite ferroelectrics. – Ibid., p. 258-268.

282. Piskunov S., Evarestov R.A., Kotomin E.A., Eglitis R., and Borstel G. Large scale first-principles calculations of Fe-doped $SrTiO_3$. – Ibid., p. 276-284.

283. Herschend B., Hermansson K., Alfredson M., Zhukovskii Yu.F., Kotomin E.A., and Jacobs P.W.M. Characterization of Metal-Ceramic Bonding in the Ag/MgO Interface from ab initio Calculations. – J. of Physical Chemistry B, 2003, **107**, p. 11893-11899.

284. Kotomin E.A., Eglitis R.I., Borstel G., and Jacobs P.W.M. Modelling of Point Defects, Polarons and Excitons in Ferroelectric Perovskites. – Proc. NATO ASI on *Computational Materials Science, Il Ciocco, Italy, 9-22 September 2001; Kluwer, Amsterdam, Berlin, Oxford,2003*, p. 291-308.

285. Evarestov R.A., Piskunov S., Kotomin E.A., and Borstel G. Single Impurities in Insulators: *Ab initio* Study of Fe-doped $SrTiO_3$. – Phys. Rev. B, 2003, **67**, 064101, 9 pages.

286. Gunhold A., Beuermann L., Goemann K., Borchardt G., Kempter V., Maus-Friedrichs W., Piskunov S., Kotomin E.A., and Dorfman S. Study of the electronic and atomic structure of thermally treated $SrTiO_3$ (110) surfaces. – Surf. and Interface Analysis, 2003, **35**, p.998-1003.

287. Kotomin E.A., Maier J., Zhukovskii Yu.F., Fuks D., and Dorfman S. *Ab initio* Modelling of Silver Adhesion on the Corundum (0001) Surface. – (Proc. EMRS, Symp. Q, Strasburg, June 18-21, 2002), Mater. Sci and Eng. C, 2003, **23**, p. 247-252.

288. Eglitis R.I., Heifets E., Kotomin E.A., Maier J., and Borstel G. First-principles Calculations for Perovskite Thin Films. – Ibid., Symp. P, Materials Science and Semiconductor Procesing, 2003, **5**, p. 129-134.

289. Eglitis R., Fuks D., Dorfman S., Kotomin E.A., and Borstel G. Large-scale Modelling of the Phase Transitions in KTN Perovskite Solid Solutions. – Ibid., Symp. P, p. 153-157.

290. Eglitis R., Kotomin E.A., G. Borstel, Kapphan S.E.,and Vikhnin V.S. Semi-empirical Calculations of the Electronic and Atomic Structure of Polarons and Excitons in ABO_3 Perovskite Crystals. – Ibid., symp. A. Computational Materials Science, 2003, **27**, p. 81-86.

291. Zvejnieks G., Kuzovkov V.N., Kotomin E.A., Zhukovskii Yu., Fuks D., Dorfman S., and Stoneham A.M. The kinetic MC modelling of reversible pattern formation in initial stages of thin metallic film growth on crystalline substrates. – Solid State Comm., 2003, **125**, p. 463-467.

292. G. Borstel, R. Eglitis, E.A. Kotomin, and E. Heifets. Modelling of Defects and Surfaces in Perovskite Ferroelectrics. – Phys. stat. sol.(b) 2003, **236**, p. 253-264.

293. R.A. Evarestov, E.A. Kotomin, E. Heifets, J. Maier, and G. Borstel. Ab initio Hartree–Fock Calculations of $LaMnO_3$ (110) Surfaces. – Sol. St. Comm., 2003, **127**, p.367-371.

294. Kotomin E.A. and Zhukovskii Yu. Ab initio Modelling of Metal Adhesion to Ceramics with Surface Defects. – In: Defects and Diffusion in Ceramics, An Annual Retospective V (Invited paper), Defects and Diffusion Forum, 2003, **218-220**, p. 67-78.

295. Eglitis R.A., Kotomin E.A., Borstel G., and Vikhnin V.S. Quantum Chemical Modelling of Electron and Hole Polarons in ABO_3 Perovskites. – In: *Fundamental Physics of Ferroelectrics 2003* (Williamsburg Int. Workshop, eds. P.K. Davies, D. Singh), AIP Conf. Proc., 2003, **677**, p. 204-209.

296. Heifets E., Eglitis R., Kotomin E.A., Goddard III W.A., Borstel G.. Calculations of perovskite polar surface structures. – Ibid., p.210-219.

297. Eglitis R., Fuks D., Dorfman S., Kotomin E.A., Borstel G. and Trepakov V. Large scale quantum chemical modelling of the phase transitions in KTN solid solutions. – Ibid., p. 231-240.

298. Kotomin E.A., Heifets E., Maier J., Goddard W. A., Atomistic simulations of $LaMnO_3$ polar surface. – Phys.Chem.Chem.Phys., 2003, **5**, p.4180-4184.

2004

299. Kotomin E.A., E.Heifets, Dorfman, D.Fuks, A. Gordon and J.Maier. Comparative study of polar perovskite surfaces. – Surface Science, 2004, **566-568**, p. 231-235. (Proc. Int. Conf. on Surface Science (ECOSS-22), Prague, September 2003).

300. Zhukovskii Yu., Kotomin E.A., Fuks D., Dorfman S. First principles simulations of the regular Cu/MgO(001) interface, Surface Science, 2004, **566-568**, p. 122-129.

301. Zhukovskii Yu., Kotomin E.A., Fuks D., and Dorfman S. A comparative study of Ag and Cu adhesion on an MgO (001) surface. – Superlattices and Microstructures, 2004, **36**, 63-72. (Proc. EMRS-2004, Symp. T).

302. E. Heifets, R. Eglitis, E.A. Kotomin, W.A. Goddard III, and G. Borstel. Ab initio calculations of the $SrTiO_3$ (110) polar surfaces. – Phys. Rev. B, 2004, **69**, 035408 (7 pp.)

303. Yu.F. Zhukovskii, E.A. Kotomin, D. Fuks, S. Dorfman, and Stoneham A.M. Adhesion trends and growth mode of ultra-thin copper films on MgO. – J.Phys: Cond. Matter, 2004, **16**, p.4881-4896.

304. Heifets E., Evarestov R.A., Kotomin E.A., Dorfman S., and Maier J. Atomistic modelling of polar $LaMnO_3$ surfaces. – Sensors and Actuators, 2004 (Proc. 20th EMRS Spring Meeting, Strasburg, Symp. N), **B 100**, p. 81-87.

305. Zhukovskii Yu., Kotomin E.A., Fuks D., Dorfman S., Stoneham A.M., Sychev O., and Borstel G. First principles simulations of 2D Cu superlattices on MgO (001) surface. – Applied Surf. Sci., 2004, **226**, p. 298-305. (Proc. 20th EMRS Spring Meeting, Strasburg, 2003.)

306. Grigorjeva L., Millers D., Pankratov V., Williams R.T., Eglitis R., Kotomin E.A., and Borstel G. Experimental and Theoretical Studies of Polaron Optical Properties in $KNbO_3$ Perovskite. – Solid State Communications, 2004, **129**, p. 691-696.

307. Zhukovskii Yu., Kotomin E.A. and Borstel G. Adsorption of single Ag and Cu atoms on regular and defective MgO (100) substrates: an ab initio study. – Vacuum, 2004, **74**, p. 235-240.

308. Eglitis R., Kotomin E.A., Borstel G. Large scale computer modelling of point defects, polarons and perovskite solid solutions. – Defect and Diffusion Forum, 2004, **226-228**, pp.169-180.

309. Eglitis R., Kotomin E.A., and Borstel G. Computer modelling of point defects in ABO_3 perovskites and MgO. – Comp. Mater. Sci., 2004, **30**, pp. 376-382. (Proc. 2nd Int. Conf. on Materials for Advanced Technologies, Singapore, December 2003)

310. R.I. Eglitis, S. Piskunov, E. Heifets, E.A.Kotomin, and G. Borstel. Ab initio study of $SrTiO_3$, $BaTiO_3$ and $PbTiO_3$ surfaces. – Ibid., Ceramics International, 2004, **30**, 1989-1992.

311. Evarestov R.A., Kotomin E.A., Fuks D., Felsteiner J., and Maier J. Ab initio calculations of the $LaMnO_3$ surface properties. – Appl. Surf. Science, 2004, **238**, p. 457-463. (Proc. APHYS-2003 conference, Spain).

312. Sychev O., Zhukovskii Yu., Kotomin E.A., and Borstel G. Ab initio calculations of copper nanostructures on MgO substrates. – Solid State Phenom. (Trans Tech Publ.), 2004, **99-100**, p. 219-223.

313. Fuks D., Dorfman S., Felsteiner J., Bakaleinikov L., Gordon A., Kotomin E.A. Ab initio calculations of atomic and electronic structure of $LaMnO_3$ and $SrMnO_3$. – Solid State Ionics, 2004, **173**, 107-111. (Proc. EMRS-04, Symp.K).

2005

314. Evarestov R.A., Bandura A.V., Alexandrov V.E., Kotomin E.A. DFT LCAO and plane wave calculations of $SrZrO_3$ perovskite. – Phys. Stat. Sol.(b), 2005, **242**, No 2, R11-13.

315. Eglitis R., Kotomin E.A. and Borstel G. Large scale computer modelling of point defects in ABO_3 perovskites. – Phys. Status Solidi, 2005, **C 2**, No 1, pp.113-119. (Proc. ICDIM-2004, Riga, July 2004.)

316. Carrasco J., Illas F., Lopez N., Kotomin E., Zhukovskii Yu., Piskunov S., Maier J., and Hermansson K. First principles simulations of F centers in $SrTiO_3$ perovskite. – Ibid., p.153-158.

317. Zhukovskii Yu. and Kotomin E.A. Transition metal adsorption on defective MgO (001) surface: ab initio study. – Ibid., p. 347-350.

318. Piskunov S., Kotomin E.A., Heifets E., Maier J., Eglitis R., Borstel G. Ab initio DFT-HF hybrid calculations of the atomic and electronic structure for ABO_3 perovskite (001) surface.– Cond. Matter Arxiv, cond.mat/0405463

319. Fuks D., Dorfman S., Piskunov S., and Kotomin E.A. Ab initio Thermodynamics of $BaSrTiO_3$ Solid Solutions. – Phys. Rev. B, 2005, **71**, 014111 (9 pages).

320. Zhukovskii Yu.F., Kotomin E.A., Mastrikov Yu., Maier J. *Ab initio* simulations on AgCl(111) surface and $AgCl(111)/Al_2O_3$ (0001) interface. – Comp. Mater. Sci., 2005, **33**, pp.276-281. (Proc. EMRS, Symp. H).

321. Piskunov S., Kotomin E.A., Fuks D., Dorfman D. Ab initio calculations of the atomic and electronic structure of layered $Ba_{0.5}Sr_{0.5}TiO_3$ structures. – Mater. Sci. Eng. B, 2005, **B 118**, 15-18.

322. Kotomin E.A., Evarestov R.A., Mastrikov Yu., and Maier J. DFT plane wave calculations of the atomic and electronic structure of $LaMnO_3$ (001) surface. – Phys.Chem.Chem.Phys., 2005, **7**, pp.2346-2350.

323. Dorfman S., Piskunov S., Kotomin E.A., and Fuks D. Electronic Properties of Layered (BaSr)TiO_3 Heterostructure. – Physica Scripta, 2005, **T 118**, pp. 276-279.

324. Zhukovskii Yu., Fuks D., Kotomin E.A., Dorfman S. *Ab initio* thermodynamics for the growth of ultra-thin Cu film on a perfect MgO (001) surface. – Mater. Sci. Eng. C (Proc. Spring EMRS, Strasbourg, 2004), 2005, **25**, p. 713-717.

325. Evarestov R.A., Kotomin E.A., Mastrikov Yu.A., Gryaznov D., Heifets E., and Maier J. Comparative density-functional LCAO and plane-wave calculations of $LaMnO_3$ surfaces. - Phys. Rev. B, 2005, **72**, 214411 (p. 1-12).

326. Piskunov S., Heifets E., Kotomin E.A., Maier J., Eglitis R.I., and Borstel G., Hybrid DFT calculations of the atomic and electronic structure for ABO_3 perovskite (001) surfaces. - Surf. Sci., 2005, **575**, p. 75-88.

327. Zhukovskii Yu.F., Piskunov S., Kotomin E.A., Sychev O., and Borstel G., *Ab initio* modelling of copper adhesion on regular $BaTiO_3$ (001) surfaces. - Microelectronic Eng., (Proc. Microelectronics Symposium, Cracow, 2004), **81**, 2005, p. 467-471.

328. Piskunov S., Kotomin E.A., and Heifets E., The electronic and atomic structure of $SrTiO_3$, $BaTiO_3$, and $PbTiO_3$ (001) surfaces: *Ab initio* DFT/HF hybrid calculations. - ibid, 2005, p. 472-477.

329. Piskunov S., Dorfman S., Fuks D., and E.A. Kotomin, BacSr1-cTiO3 perovskite solid solutions: Thermodynamics from ab initio electronic structure calculations. - ibid, 2005, p. 478-484.

330. Kotomin E.A., Evarestov R.A., Mastrikov Yu.A., and Maier J. DFT plane wave calculations of the atomic and electronic structure of $LaMnO_3$ (001) surface. - Phys. Chem. and Chem. Phys., 2005, **7**, p. 2346-2350.

331. Zhukovskii Yu.F., Kotomin E.A., Mastrikov Yu.A., and Maier J. Ab initio simulations on AgCl(111) surface and AgCl(111)/a-Al2O3(0001) interface. - Comput. Mater. Sci., 2005, **33**, p. 276-281.

332. Piskunov S., Kotomin E.A., Fuks D., and Dorfman S. Ab initio calculations of the atomic and electronic structure of layered $Ba_{0.5}Sr_0.5TiO_3$ structures . - Mater. Sci. and Eng. B (Proc. Spring EMRS, Strasbourg, 2004), 2005, **118**, p. 15-18.

333. Dorfman S., Piskunov S., Kotomin E.A., and Fuks D. Electronic properties of layered $Ba_{0.5}Sr_{0.5}TiO_3$ heterostructure: ab initio hybrid density functional calculations. - Phys. Scripta (Proc. Int. Meeting on Applied Physics, Badajos, 2003), 2005, **T118**, p. 276-279.

2006

334. Kotomin E.A. and Popov A.I. The kinetics of radiation-induced point defect aggregation and metallic colloid formation in ionic solids. In: Radiation Effects in Solids, NATO ASI Science Series II. Physics, Chemistry and Mathematics (Eds. K. Sikafus and E.A. Kotomin), Vol. **235**, p. 153-192.

335. Zhukovskii Yu.F., Balaya P., Kotomin E.A., and Maier J. Evidence for interfacial-storage anomaly in nanocomposites for lithium batteries from first-principles simulations. - Phys. Rev. Letters, 2006, **96**, 058302 (p. 1-4).

336. Carrasco J., Illas F., Lopez N., Kotomin E.A., Zhukovskii YU.F., Evarestov R.A., Mastrikov Yu.A., Piskunov S., and Maier J. First principles calculations of atomic and electronic structure of F center in bulk and on the (001) surface of $SrTiO_3$. - Phys. Rev. B, 2006, **73**, 064106 (p.1-12)

337. Fuks D., Kotomin E.A., Zhukovskii Yu.F., and Stoneham A.M. The size and shape of 3D Cu clusters on MgO(001) substrate: combined *ab initio* and thermodynamic calculations. - Phys. Rev. B, 2006, **74**, 115418 (p.1-6).

338. Krischok S., Stracke P., Hoefft O., Kempter V., Zhukovskii Yu.F., and Kotomin E.A. A comparative analysis of electron spectroscopy and first principles studies on Cu(Pd) adsorption on MgO. - (Proc. ECOSS-23 Conf., Berlin, 2005) Surf. Sci., 2006, **600**, p.3815-3820.

339. Fuks D., Zhukovskii Yu.F., Kotomin E.A., and Ellis D.E. Metal film growth on regular and defective MgO(001) surface: A comparative *ab initio* simulation and thermodynamic study. - Surf. Sci., 2006, **600**, p.L99-104.

340. Evarestov R.A., Kotomin E.A., and Zhukovskii YU.F. DFT study of a single *F*-center in cubic $SrTiO_3$ perovskite. - Intern. J. Quant. Chem., 2006, **106**, p.2173-2183.

341. Jamnik J., Kalnin J.R., Kotomin E.A., and Maier J. Generalised Maxwell-Garnett equation: application to electrical and chemical transport. - Phys. Chem. and Chem. Phys, 2006, **8**, 1310-1314.

342. Heifets E., Kotomin E.A., and Trepakov V.A. Calculations for antiferrodistortive phase of $SrTiO_3$ perovskite: hybrid density functional study. - J. Phys.: Cond. Matter, 2006, **18**, p. 4845-4851

343. Eglitis R.I., Borstel G., Heifets E., Piskunov S., and Kotomin E.A. Ab initio calculations of the $BaTiO_3$ (100) and (110) surfaces. - J. Electroceram., 2006, **16**, p. 289-292.

344. Fuks D., Bakaleinikov L., Kotomin E.A., Felsteiner J., Gordon A., Evarestov R.A., Gryaznov D., and Maier J. Thermodynamic stability and disordering in LacSr1-cMnO3 solid solutions. - Solid State Ionics (Proc. 15th Int. Conference SSI'2005, Baden-Baden, 2005), 2006, **177**, p. 217-222.

345. Galinetto P., Rossella F., Samoggia G., Trepakov V.A., Kotomin E.A., Heifets E., Markovin P., and Jastrabik L. Structural phase transition and photo-charge carrier transport in $SrTiO_3$. - Ferroelectrics (Proc. 11th Int. Meeting on Ferroelectricity, Foz do Iguacu, Brasil, 2005), 2006, **337**, p. 179-188.

346. Balaya P., Bhattacharyya A.J., Jamnik J., Zhukovskii Yu.F., Kotomin E.A., and Maier J. Nano-ionics in the context of lithium batteries. - J. Power Sources, 2006 (Proc. Int. Conf. Materials for Advanced Technologies, Singapore, 2005), **159**, p. 171-178.

347. Piskunov S., Kotomin E.A., Zhukovskii Yu.F., Heifets E., and Ellis D.E. Adsorption of atomic and molecular oxygen on the $SrTiO_3$ (001) surfaces: Predictions by means of hybrid density functional calculations. - MRS Proc. (Fall MRS, Boston, MA, 2005), 2006, **894**, LL08-05 (p. 1-6).

348. Kotomin E.A., Zhukovskii Yu.F., Mastrikov Yu.A., and Maier J. First-Principles modeling of oxide surfaces and their reactivity. - Latv. Journ. Phys. and Tech. Sci.

(Proc. 2nd FMNT conference, Riga, Latvia, 2006), 2006, **No 2**, p. 127-140.

2007

349. Heifets E., Piskunov S., Kotomin E.A., Zhukovskii Yu.F., and Ellis D.E. Electronic structure and thermodinamic stability of double-layered $SrTiO_3$ (001) surfaces: Ab initio simulations. - Phys. Rev. B, 2007, **75**, 115417 (13 p.)

350. Piskunov S., Gopejenko A., Kotomin E.A., Zhukovskii Yu.F., and Ellis D.E. Atomic and electronic structure of perfect and defective $PbZrO_3$ perovskite: hybrid DFT calculations of cubic and orthorhombic phases. - Comput. Mater. Sci., 2007, **41**, p.195-201.

351. Kotomin E.A., Mastrikov Yu., Zhukovskii Yu.F., Van Uffelen P., and Rondinella V.V. First-principles modelling of defects in advanced nuclear fuels. - Physica Status Solidi C (Proc. 10th EURODIM, Milano, 2006), 2007, **C4**, p. 1193-1196.

352. Zhukovskii Yu.F., Fuks D., Kotomin E.A., and Ellis D.E. Differences in the metallic film growth mode on perfect and defective MgO surfaces. - Nucl. Instr. Meth., 2007, **B 255**, p.219-222 (Proc. 8th Int. Conf. COSIRES-8, Richland, WA, 2006).

353. Kotomin E.A., Grimes R.W., Mastrikov Yu., and Ashley N.J. Atomic scale DFT simulations of point defects in uranium nitride. - J. Phys.: Cond. Matter, 2007, **19**, 106208 (p. 1-9).

354. Piskunov S., Spohr E., Jacob T., Kotomin E.A., Ellis D. Electronic and magnetic structure of $LaSrMnO_3$ calculated by means of hybrid density functional theory. - Phys. Rev. B, 2007,**76**, 12410 (4 p.)

355. Vracar M., Kuzmin A., Merkle R., Purans Yu., Kotomin E.A., Maier J., Mathon O. Structural studies of $Sr(Ti,Fe)O_3$ solid solutions by XAS, XRD and vibrational spectroscopy. – Phys. Rev. B, 2007, **76**, p. 174107 (12 p.)

356. Zhukovskii Yu.F., Balaya P., Dolle M., Kotomin E.A., and Maier J. Enhanced lithium storage and chemical diffusion in metal-LiF nanocomposties: Experimental and theoretical results. – Phys. Rev. B, 2007, **76**, p. 235414 (6 p.)

2008

357. Kotomin E.A., Gryaznov D., Grimes R.W., Parfitt D., Zhukovskii Yu.F., Mastrikov Yu., Van Uffelen P., Rondinella V., Konings R. First-principles modelling of radiation defects in advanced nuclear fuels. - Nucl. Inst. Meth. B, 2008, **266**, 2671 (Proc. REI-14, Caen, August 2007).

358. Zhukovskii Yu.F., Kotomin E.A., Balaya P., and Maier J. Enhanced interfacial lithium storage in nanocomposites of transition metals with LiF and Li_2O. – Solid State Science, 2008, **10**, 491.

359. Zhukovskii Yu.F., Kotomin E.A., and Ellis D.E. A comparative ab initio study of Cu overlayers on $BaTiO_3$ (001) and MgO (001) substrates. – Phys. stat. sol. (b), 2008, **245**, 980.

360. Kotomin E.A., Mastrikov Yu., Heifets E., and Maier J. Adsorption of atomic and molecular oxygen on the $LaMnO_3$ (001) surface: ab initio supercell calculations and thermodynamics. – Phys.Chem. Chem.Phys., 2008, **10**, 4644; arxiv cond.mat. 2008-0802-0193v2.

361. E. A. Kotomin, Yu. F. Zhukovskii, S. Piskunov, and D. E. Ellis. Hybrid DFT calculations of the F centers in cubic ABO_3 perovskites. – J.Phys.: Conf. series, 2008, **117** 012019 (6 pp.) (Int. Workshop on Ab initio Simulations of Crystalline Solids, Torino, Italy.)

362. V.E. Alexandrov, R.A. Evarestov, E.A. Kotomin and J. Maier. Ab initio study of bulk and surface iron defects in $SrTiO_3$. – Ibid., p. 012001 (6 pp.)

363. E.A. Kotomin, Yu.A. Mastrikov, E. Heifets, R. Merkle, J. Fleig, J. Maier, A. Gordon and J.Felsteiner. First principles modeling of SOFC cathode – Proc. Electrochemical Society, 2008, **13**, 301.

364. E.A. Kotomin and Yu.A. Mastrikov, First principles modelling of oxygen impurities in UN nuclear fuels. – J. Nucl. Mater., 2008, **377**, 492.

365. E. A. Kotomin, S. Piskunov, Yu. F. Zhukovskii, R. I. Eglitis, A. Gopejenko, and D. E. Ellis. The electronic properties of oxygen vacancy at ZrO_2-terminated (001) surfaces of cubic $PbZrO_3$: Computer simulations from the first principles. – Phys.Chem. Chem.Phys., 2008, **10**, 4258.

366. R.A. Evarestov, A.V. Bandura, M.V. Losev, E.A. Kotomin, Yu.F. Zhukovskii, and D. Bocharov. A first-principles DFT study of UN bulk and (001) surface: comparative LCAO and PW calculations. – J. Comp. Chem., 2008, **29**, 2079.[Special volume on solid state chemistry.]

367. Piskunov S., Heifets E., Jacob T., Kotomin E.A., Ellis D., Spohr E. Electronic structure and thermodynamic stability of $LaMnO_3$ and LSM. – Phys. Rev. B, 2008, **78**, 121406.

368. Alexandrov V., Kotomin E.A., Maier J., and Evarestov R.A. Ab initio modelling of spin and charge ordering and lattice dynamics in $CaFeO_3$ crystals. – J. Chem. Phys., 2008, **129**, 214704.

2009

369. Mastrikov Yu., Heifets E., Kotomin E.A., and Maier J. Atomic, electronic and thernodynamic properties of cubic and orthorhombic $LaMnO_3$ surfaces. – Surf. Sci., 2009, **603**, 326-335.

370. Zhukovskii Yu.F., Kotomin E.A., Piskunov S., and Ellis D.E. A comparative ab initio study of bulk and surface oxygen vacancies in $PbTiO_3$, $PbZrO_3$ and $SrTiO_3$ perovskites. - Solid State Commun., 2009, **149**, 1359-1362.

371. Zhukovskii Yu.F., Bocharov D., and Kotomin E.A. Chemisorption of a molecular oxygen on the UN (001) surface: ab initio calculations. - J. Nucl. Mater., 2009, **393**, 504-507.

372. Zhukovskii Yu.F., Bocharov D., Kotomin E.A., Evarestov R.A. and Bandura A.V. First principles calculations of oxygen adsorption on the UN (001) surface. - Surf. Sci., 2009, **603**, 50-53.

373. Kotomin E.A., Mastrikov Yu.A., Rashkeev S., van Uffelen P. Implementing first principles calculations of defect migration in a fuel performance code for UN simulations. - J. Nucl. Mater., 2009,**393**, 292-299 .

374. Zhukovkii Yu.F., Kotomin E.A., Piskunov S., Mastrikov Yu.A., and Ellis D.E. The effect of oxygen vacancies on the atomic and electronic structure of cubic ABO3 perovskite bulk and the (001) surface: Ab initio calculations. - Ferroelectrics (Proc. 9th Int. Symp. on Ferroelectricity, Vilnius, Lithuania, 2008), 2009, **379**, 191-198.

375. Gryaznov D., Heifets E., and Kotomin E.A. Ab initio DFT+U study of He atom incorporation into UO_2 crystals. - PCCP, 2009, **11**, 7241-7247.

376. Alexandrov V., Kotomin E.A., Maier J., and Evarestov R.A. First-principles study of bulk and surface oxygen vacancies in $SrTiO_3$ crystal. - Eur. Phys. J. B, 2009, **72**, 53-57.

377. Merkle R., Mastrikov Yu., Heifets E., Kotomin E.A., Kuklja M., and Maier J. Oxygen incorporation reaction into mixed conducting perovskites: a mechanistic analysis for (La,Sr)MnO_3 based on DFT calculations. - Elect. Chem. Soc. Trans., 2009, **25**, 2753-2760.

2010

378. Mastrikov Yu.A., Merkle R., Heifets E., Kotomin E.A., and Maier J. Pathways for Oxygen Incorporation in Mixed Conducting Perovskites: A DFT-Based Mechanistic Analysis for (La,Sr)MnO_3.– J. Phys. Chem. C, 2010, **114**, 3017-3027.

379. Vassilyeva A.F., Eglitis R.I., Kotomin E.A., Dauletbekova A.K. Ab initio calculations of MgF_2 (001) and (011) surface structure. – Physica B, 2010, **405**, 2125-2127.

380. Eglitis R.I., Kotomin E.A. Ab initio calculations of Nb doped $SrTiO_3$. – Physica B, 2010, **405**, 3164-3168.

381.Mastrikov Yuri A., Kuklja Maija M., Kotomin Eugene A., and Maier Joachim. First-principles modelling of complex perovskite $(Ba_{1-x}Sr_x)(Co_{1-y}Fe_y)O_3$- for solid oxide fuel cell and gas separation membrane applications.– Energy and Environmental Science, 2010, **3**, 1544-1549.

382. Kuzovkov V.N., Zvejnieks G., Kotomin E.A., Olvera de la Cruz M. Microscopic approach to the kinetics of pattern formation of charged molecules on surfaces. – Phys. Rev. E, 2010, **82**, 021602 (10 pp.)

383. Popov A.I., Kotomin E.A., Maier J. Basic properties of the F-type centers in halides, oxides and perovskites. – Nucl. Inst. Meth. B, 2010, **268**, 3084-3089.

384. Kuzovkov V.N., Kotomin E.A., Merzlyakov P., Zvejnieks G., Li K.D., Ding T.H., Wang L.M. Void superlattice formation in electron irradiated CaF_2: Theoretical analysis. – Nucl. Inst. Meth. B, 2010, **268**, 3055-3058.

385. Gryaznov D., Rashkeev S., Kotomin E.A., Heifets E., Zhukovskii Yu. Helium behaviour in oxide nuclear fuels: First principles modeling. – Nucl. Inst. Meth. B, 2010, **268**, 3090-3094.

386. Gopejenko A., Zhukovskii Yu.F., Vladimirov P.V., Kotomin E.A., and Moeslang A. Ab initio simulation of yttrium oxide nanocluster formation on fcc Fe lattice. - J. Nucl. Mater., 2010, **406**, 345-350.

2011

387. Kotomin E.A., Alexandrov V., Gryaznov D., Evarestov R.A., Maier J. Confinement effects for ionic carriers in $SrTiO_3$ ultrathin films: first-principles calculations of oxygen vacancies. – Phys Chem Chem Phys, 2011, **13**, 923-926.

388. Bocharov D., Gryaznov D., Zhukovskii Yu.F., Kotomin E.A. DFT calculations of point defects on UN (001) surface. – Surf. Sci., 2011,**605** , 396-400.

389. Bocharov D., Gryaznov D., Zhukovskii Yu.F., Kotomin E.A. Ab initio modelling of oxygen impurity incorporation into uranium mononitride surface and sub-surface vacancies. – J. Nucl. Mater., 2011, **416**, 200-204

390. Kotomin E.A., Mastrikov Yu., Kuklja M.M., Merkle R., Maier J. First principles calculations of oxygen vacancy formation and migration in mixed conducting BSCF perovskites. – Solid State Ionics, 2011, **188** , 1-5.

391. Vassilyeva A., Eglitis R., Kotomin E.A., Dauletbekova A. Ab initio calculations of the atomic and electronic structure of MgF_2 (011) and (111) surfaces. – Centr. Eur. J. Phys., 2011, **9**, 515-518.

392. Evarestov R.A., Blokhin E., Gryaznov D., Kotomin E.A., Maier J. Phonon calculations in cubic and tetragonal phases of $SrTiO_3$: a comparative LCAO and plane wave study. – Phys. Rev. B, 2011, **83**, 134108 (pp.1-9).

393. Zhukovskii Yu.F., Piskunov S., Kotomin E.A., and Bellucci. Simulations on the mechanism of CNT bundle growth upon smooth and nanostructured Ni as well as gamma-Al_2O_3 catalysts. – Centr. Eur. J. Phys., 2011, **9**, 530-541.

394. Blokhin E., Gryaznov D., Kotomin E., Evarestov R.A., Maier J. A comparative hybrid DFT study of phonons in several $SrTiO_3$ phases. – Intergated Ferroelectrics, 2011, **123**, p. 18-25

395. Kotomin E.A., Merkle E., Mastrikov Yu,, Kuklja M.M., and Maier J. First Principles Modeling of Oxygen Mobility in Perovskite SOFC Cathode and Oxygen Permeation Membrane Materials – ECS Transactions, 2011, **35** , 823-830.

396. Kuklja M.M., Mastrikov Yu., Rashkeev S., and Kotomin E.A. The Structural Disorder and Lattice Stability of (Ba,Sr)(Co,Fe)O_3 Complex Perovskites. – ECS Transactions, 2011, **35**, 2077 - 2084.

397. Kuzovkov V.N., Kotomin E.A., Zvejnieks G. Pattern formation kinetics for charged molecules on surfaces: the microscopic correlation function analysis. - J Phys Chem B, 2011, **115**, 14626-35

398. Kuzovkov V.N., Kotomin E.A., M. Olvera de la Cruz, The non-equilibrium charge screening effects in diffusion-driven systems with pattern formation. – J Chem Phys, 2011, **135**, 034702 (p. 1-6).

399. Alexandrov V., Piskunov S., Zhukovskii Yu.F., Kotomin E.A., and Maier J., First-Principles Modeling of Oxygen Interaction with SrTiO3(001) Surface: Comparative Density-Functional LCAO and Plane-Wave Study, Integrated Ferroelectrics, 2011, **123**, pp. 10-17.

400. Gopejenko A., Zhukovskii Yu.F., Vladimirov P.V., Kotomin E.A., and Moeslang A. Modeling of yttrium, oxygen atoms and vacancies in α -iron lattice. - J. Nucl. Mater., 2011, **416**, p. 40-44.

401. V.N. Kuzovkov, E.A. Kotomin, and G. Zvejnieks, Atomistic theory of mesoscopic pattern formation induced by bimolecular surface reactions between oppositely charged molecules. - J. Chem. Phys., 2011, **135**, 224503 (p. 1-5)

2012

402. Merkle R., Mastrikov Yu.A., Kotomin E.A., Kuklja M.M., Maier J., First principles calculations of oxygen vacancy formation and migration in Ba1-xSrxCo1-yFeyO3 perovskites. - J. Electrochem. Soc., 2012, **159**, p. B219-B226.

403. A.V. Sorokin, Yu.F. Zhukovskii, J. Purans, and E.A. Kotomin, The effect of Zn vacancies and Ga dopants on the electronic structure of ZnO: Ab initio simulations. - IOP Conf. Series: Mater. Sci. Engineering, 2012, **38**, 012015 (p. 1-4).

404. F.U. Abuova, A.T. Akilbekov, and E.A. Kotomin, Ab initio calculations of the H centers in MgF_2 crystals. - IOP Conf. Series: Mater. Sci. Engineering, 2012, **38**, 012041 (p. 1-4)

405. E.A. Kotomin, Yu.F. Zhukovskii, D. Bocharov, and D. Gryaznov, Ab initio modelling of UN grain boundary interfaces. - IOP Conf. Series: Mater. Sci. Engineering, 2012, **38**, 012058 (p. 1-4).

406. R.A. Evarestov, E. Blokhin, D. Gryaznov, E.A. Kotomin, R. Merkle, and J. Maier, Jahn-Teller effect in the phonon properties of defective $SrTiO_3$ from first principles. - Phys. Rev. B, 2012, **85**, 175303 (p.1-5).

407. D. Gryaznov, E. Heifets, and E.A. Kotomin, The first-principles treatment of the electron-correlation and spin-orbital effects in uranium mononitride nuclear fuels. - Phys. Chem. Chem. Phys., 2012, **14**, p. 4482-4490.

408. E. Blokhin, E.A. Kotomin, and J. Maier, First-principles phonon calculations of Fe^{4+} impurity in $SrTiO_3$. - J. Phys.: Condens. Matter, 2012, **24**, 104024 (p. 1-4).

409. J.R. Kalnin and E.A. Kotomin, Note: Effective diffusion coefficient in heterogeneous media. - J. Chem. Phys., 2012, **137**, 166101 (p. 1-2).

410. M.M. Kuklja, Yu.A. Mastrikov, B. Jansang, and E.A. Kotomin, The Intrinsic Defects, Disordering, and Structural Stability of $Ba_xSr_{1-x}Co_yFe_{1-y}O_3$ Perovskite Solid Solutions. - J.Phys.Chem. C, 2012, **116**, p. 18605-18611.

411. A.F Fix, F.U. Abuova, R.I. Eglitis, E.A. Kotomin, and A.T. Akilbekov, Ab initio calculations of the F centers in MgF_2 bulk and on the (001) surface. - Phys. Scr., 2012, **86**, 035304 (p. 1-5).

412. Abuova F., Useinov A., Akilbekov A.T., Kotomin E.A., Piskunov S., and Lisitsyn V.M. First-principles calculations of radiation defects in magnesium fluorite. – Izv. vuzov fizika (Russian Jourtal of Physics) 2012 **55** N 11, p.9-12

2013

413. Yu.A. Mastrikov, R. Merkle, E.A. Kotomin, M.M. Kuklja, and J. Maier, Formation and migration of oxygen vacancies in $La_{1-x}Sr_xCo_{1-y}$ Fe_yO_3 perovskites: insight from ab initio calculations and comparison with $Ba_{1-x}Sr_xCo$ $_{1-y}$ Fe_yO_3. - Phys. Chem. Chem. Phys., 2013, **15**, p. 911 - 918.

414. A. Weizman, D. Fuks, E.A. Kotomin, and D. Gryaznov, Ab initio study of phase competition in $(La_{1-c},Sr_c)CoO_3$ solid solutions. - Solid State Ionics, 2013, **230**, p. 32-36.

415. M.M. Kuklja, Yu.A. Mastrikov, B. Jansang, and E.A. Kotomin, First principles calculations of (Ba,Sr)(Co,Fe)O_3 structural stability. - Solid State Ionics, 2013, **230**, p. 21-26.

416. Fuks D., Weizman A., and Kotomin E.A., Phase competition in (La,Sr) CoO_3 solid solutions: ab initio thermodynamic study. - Phys. Status Solidi B, 2013, **250**, p. 864-869.

417. Blokhin E., Kotomin E.A., Kuzmin A., Purans J., Evarestov R.A., and Maier J., Theoretical modeling of the complexes of iron impurities and oxygen vacancies in $SrTiO_3$. - Appl. Phys. Lett., 2013, **102**, 112913 (p. 1-5).

418. Dauletbekova A., Abuova F., Akilbekov A.T., Kotomin E.A., and Piskunov S., First-principles modeling of the H color centers in MgF_2 crystals. - Phys. Status Solidi C, 2013, **10**, p. 160-164. (Proc. ICDIM conference Santa Fe, 2012).

419. Bocharov D., Gryaznov D., Zhukovskii Yu.F., and Kotomin E.A., Ab initio simulations of oxygen interaction with surfaces and interfaces in uranium mononitride. - J. Nucl. Mater., 2013, **435**, p. 102-106.

420. Gryaznov D., Blokhin E., Sorokin A., Kotomin E.A., Evarestov R.A., Bussmann-Holder A., and Maier J., A comparative ab initio thermodynamic study of oxygen vacancies in ZnO and $SrTiO_3$: emphasis on phonon contribution. - J. Phys. Chem. C, 2013, **117**, p. 13776-13784.

421. D. Fuks, Yu. Mastrikov, E.A. Kotomin, and J. Maier, Ab initio thermodynamic study of (Ba,Sr)(Co,Fe)O3 perovskite solid solutions for fuel cell applications. - J. Mater. Chem. A, 2013, **1**, p. 14320-14328.

422. M.M. Kuklja, E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, and J. Maier. Combined theoretical and experimental analysis of processes determining cathode performance in solid oxide fuel cells. - Phys. Chem. Chem. Phys., 2013, **15**, 5443-5471.

423. E. Blokhin, R.A. Evarestov, D. Gryaznov, E.A. Kotomin, and J. Maier. Theoretical modeling of antiferrodistortive phase transition for $SrTiO_3$ ultrathin films. - Phys. Rev. B, 2013, **88**, 241407 (p. 1-4).

424. A. Usseinov, E.A. Kotomin, Yu.F. Zhukovskii, J. Purans, A. Sorokin, and A.T. Akilbekov. Atomic and electronic structure of hydrogen on ZnO (1-100) surface: ab initio hybrid calculations. - IOP Conf. Series: Mater. Sci. Engineering, 2013, **49**, 012054 (p. 1-4).

2014

425. A.B. Usseinov, E.A. Kotomin, A.T. Akilbekov, Yu F. Zhukovskii, and J. Purans. Hydrogen induced metallization of ZnO (1-100) surface: Ab initio study. - Thin Solid Films, 2014, **553**, 38-42.

426. G. Zvejnieks, V.N. Kuzovkov, and E.A. Kotomin, Statistical characterization of self-assembled charged nanoparticle structures. - Phys. Status Solidi A, 2014, **211**, 288-293.

427. M.M. Kuklja, E.A. Kotomin, O. Sharia, Yu.A. Mastrikov, and J. Maier, Radiation defects in complex perovskite solid solutions. - Nucl. Instrum. Meth. B., 2014, **326**, 243-246.

428. F.U. Abuova, E.A. Kotomin, V.M. Lisitsyn, A.T. Akilbekov, and S. Piskunov, Ab initio modeling of radiation damage in MgF_2 crystals. - Nucl. Instrum. Meth. B., 2014, **326**, 314-317

429. A.B. Usseinov, E.A. Kotomin, A.T. Akilbekov, Yu.F. Zhukovskii, and J. Purans, Hydrogen adsorption on the ZnO (1100) surface: ab initio hybrid density functional linear combination of atomic orbitals calculations. - Phys. Scr., 2014, **89**, 045801 (p. 1-7)

430. V. N. Kuzovkov, G. Zvejnieks, and E. A. Kotomin Theory of non-equilibrium critical phenomena in three-dimensional condensed systems of charged mobile nanoparticles Physical Chemistry Chemical Physics , 2014, **16(27)**, 13974-13983.

431. V.N. Kuzovkov and E.A. Kotomin, Static and dynamic screening effects in the electrostatic self-assembly of nano-particles. - Phys. Chem. Chem. Phys., 2014, **16**, 25449-25460.

432. T.S. Bjorheim and E. A. Kotomin. Ab Initio Thermodynamics of Oxygen Vacancies and Zinc Interstitials in ZnO The Journal of Physical Chemistry Letters, 2014, **5**, 4238-4242.

433. D. Gryaznov, S. Baumann, E.A. Kotomin, and R. Merkle, Comparison of permeation measurements and hybrid density-functional calculations on oxygen vacancy transport in complex perovskite oxides. - J. Phys. Chem. C, 2014, **118**, 29542- 29553

2015

434. M. Arrigoni, E.A. Kotomin, D. Gryaznov, and J. Maier, Confinement effects for the F center in non-stoichiometric $BaZrO_3$ ultrathin films. - Phys. Status Solidi B, 2015, **252**, 139 - 143.

435. A. Platonenko, S. Piskunov, Yu.F. Zhukovskii, and E.A. Kotomin, Ab initio simulations on Frenkel pairs of radiation defects in corundum. - IOP Conf. Ser. Mater. Sci. Eng., 2015, **77**, 012001 (pp. 1-5).

436. G.A. Kaptagay, T.M. Inerbaev, Yu.A. Mastrikov, E.A. Kotomin, A.T. Akilbekov, Water interaction with perfect and fluorine-doped Co3O4 (100) surface. - Solid State Ionics, 2015, **277**, p. 77-82

437. J.R. Kalnin and E.A. Kotomin, The effective diffusion coefficient in a one-dimensional discrete lattice with the inclusions. - Physica B , 2015, **470-471**, p. 50-52.

438. T.S. Bjorheim, E.A. Kotomin, and J. Maier, Hydration entropy of $BaZrO_3$ from first principles phonon calculations. - J. Mater. Chem. A, 2015, **3**, p. 7639-7648.

439. A.U. Abuova, Yu.A. Mastrikov, E.A. Kotomin, Y. Kawazoe, T.M. Inerbaev, and A.T. Akilbekov, First principles modeling of Ag adsorption on the $LaMnO_3$ (001) surfaces. - Solid State Ionics, 2015, **273**, p. 46-50.

440. E. Heifets, E.A. Kotomin, A.A. Bagaturyants, and J. Maier, Ab Initio study of $BiFeO_3$: thermodynamic stability conditions. - J. Phys. Chem. Lett., 2015, **6**, p. 2847-2851

441. T. S. Bjoerheim, M. Arrigoni, D. Gryaznov, E.A. Kotomin, and J. Maier,Thermodynamic properties of neutral and charged oxygen vacancies in $BaZrO_3$ based on first principles phonon calculations- - Phys Chem Chem Phys 2015, **17**, p. 20765.

442. M. Arrigoni, E.A. Kotomin, J. Maier, Large-scale modeling of defects in advanced oxides: oxygen vacancies in $BaZrO_3$ crystals. - In a book: W.E. Nagel (ed.), High Performance Computing in Science and Engineering-2015 (Springer, Berlin), p.187-198. doi: 10.1007/978-3-319-24633-8-12.

2016

443. G. Zvejnieks, P. Merzlyakov, V.N. Kuzovkov, and E.A. Kotomin, Void lattice formation in electron irradiated CaF2: Statistical analysis of experimental data and cellular automata simulations. - Nucl. Instrum. Meth. B., 2016 **368**, p. 138-143.

444. D. Bocharov, M. Chollet, M. Krack, J. Bertsch, D. Grolimund, M. Martin, A. Kuzmin, J.Purans, and E.A. Kotomin, Interpretation of the U L3-edge EXAFS in uranium dioxide using molecular dynamics and density functional theory simulations. - J. Phys. Conf. Ser., 2016, **712**, 012013 (1-4).

445. A.I. Popov, A. Lushchik, and E.A. Kotomin, Low-temperature radiation effects in wide gap materials. - Low Temp. Phys., 2016, **42**, p. 687-688.

446. V.N. Kuzovkov, A.I. Popov, E.A. Kotomin, A.M. Moskina, E. Vasil'chenko, and A. Lushchik, Theoretical analysis of the kinetics of low-temperature defect recombination in alkali halide crystals. - Low Temp. Phys., 2016, **42**, p. 748-755.

447. M. Arrigoni, T.S. Bjoerheim, E.A. Kotomin, and J. Maier, First principles study of confinement effects for oxygen vacancies in $BaZrO_3$ (001) ultra-thin films. - Phys.Chem. Chem.Phys. Comm., 2016, **18**, p. 9902-9908.

448. V.M. Lisitsyn, L.A. Lisitsyna, A.I. Popov, E.A. Kotomin, F.U. Abuova, A. Akilbekov, and J. Maier, Stabilization of primary mobile radiation defects in MgF_2 crystals. - Nucl. Instr. Meth. Phys. Res. B, 2016, **374**, p. 24-28.

449. Yu.F. Zhukovskii, A. Platonenko, S. Piskunov, and E.A. Kotomin, Ab initio simulations on migration paths of interstitial oxygen in corundum. - Nucl. Instr. Meth. Phys. Res. B, 2016, **374**, p. 29-34.

450. E.A. Kotomin, V.N. Kuzovkov, A.I. Popov, and R. Vila, Kinetics of F center annealing and colloid formation in Al_2O_3. - Nucl. Instr. Meth. Phys. Res. B, 2016, **374**, p. 107-110.

451. Yu.A. Mastrikov, S. Guo, F. Puleo, L.F. Liotta, and E.A. Kotomin, First principles modeling of Pd-doped (La,Sr)(Co,Fe)O_3 complex perovskites. - Fuel Cells, 2016, **16**, p. 267-271.

452. T.S. Bjoerheim, M. Arrigoni, S.W. Saeed, E.A. Kotomin, and J. Maier, Surface segregation entropy of protons and oxygen vacancies in $BaZrO_3$. - Chem. Mater., 2016, **28**, p.1363 - 1368.

453. D. Gryaznov, R. Merkle, E.A. Kotomin and J. Maier, Ab initio modelling of oxygen vacancies and protonic defects in $LaSrFeO_3$ perovskite solid solutions. - J. Mater. Chem. A, 2016, **4**, 13093 - 13104.

454. A. Gopejenko, Yu.F. Zhukovskii, E.A. Kotomin, Yu.A.. Mastrikov, P.V. Vladimirov, V.A. Borodin, and A. Moeslang, Ab initio modelling of Y- O cluster formation in fcc- Fe lattice. - Phys. Status Solidi B, 2016, **253**, p. 2136 - 2143

455. A. Platonenko, D. Gryaznov, S. Piskunov, Yu. F. Zhukovskii, E. A. Kotomin, Charged oxygen interstitials in corundum: first principles simulations – Phys. Status Solidi C, 2016, **13**, p. 932 - 936

2017

456. R.A. Evarestov, D. Gryaznov, M. Arrigoni, E.A. Kotomin, A. Chesnokov and J. Maier, Use of site symmetry in supercell models of defective crystals: polarons in CeO_2. - Phys. Chem. Chem. Phys., 2017, **19**, p. 8340-8348.

457. A.I. Popov, E.A. Kotomin, and J. Maier, Analysis of self-trapped hole mobility in alkali halides and metal halides. - Solid State Ionics, 2017, **302**, p. 3-6.

458. E. Heifets, E.A. Kotomin, A.A. Bagaturyants and J. Maier, Thermodynamic stability of stoichiometric $LaFeO_3$ and $BiFeO_3$: a hybrid DFT study. - Phys. Chem. Chem. Phys., 2017, **19**, p. 3738-3755.

459. D. Bocharov, M. Chollet, M. Krack, J. Bertsch, D. Grolimund, M. Martin, A. Kuzmin, J. Purans, and E.A. Kotomin, Analysis of the U L3-edge X-ray absorption spectra in UO_2 using molecular dynamics simulations. - Progr. Nucl. Ener., 2017, **94**, p. 187-193.

460. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M.M. Kuklja, and J. Maier, The effect of (La,Sr)MnO_3 cathode surface termination on its electronic structure. - ECS Transactions, 2017, **77**, p. 67-73.

461. M. Arrigoni, E.A. Kotomin, and J. Maier, First-principles study of perovskite ultrathin films: Stability and confinement effects. - Isr. J. Chem., 2017, **57**, p.509-521.

462. R.A. Evarestov, A. Platonenko, D. Gryaznov, Yu.F. Zhukovskii, and E.A. Kotomin. First-principles calculations of oxygen interstitials in corundum: a site symmetry approach. – Phys. Chem. Chem. Phys., 2017, **19**, p. 25245-25251.

463. L.L. Rusevich, G. Zvejnieks, A. Erba, R. Dovesi, and E.A. Kotomin. Electromechanical properties of Ba(1-x)SrxTiO3 perovskite solid solutions from first-principles calculations.–J. Phys. Chem. A, 2017, **121**, p. 94099414.

2018

464. V.N. Kuzovkov, E.A. Kotomin, and A.I. Popov. Kinetics of the electronic center annealing in Al_2O_3 crystals.– J. Nucl. Mater., 2018, **502**, pp. 295-300.

465. E. Kotomin, V. Kuzovkov, A.I. Popov, J. Maier, and R. Vila. Anomalous kinetics of diffusion-controlled defect annealing in irradiated ionic solids. – J. Phys. Chem. A, 2018, **122**, pp. 2832

466. G. Zvejnieks, A. Anspoks, E.A. Kotomin, and V.N. Kuzovkov. Kinetic Monte Carlo modeling of Y_2O_3 nano-cluster formation in radiation resistant matrices. – Nucl. Instrum. Methods Phys. Res. B, 2018, **434**, pp. 13-22.

467. A.I. Popov, A. Lushchik, E. Shablonin, E. Vasilchenko, E.A. Kotomin, A.M. Moskina, and V.N. Kuzovkov. Comparison of the F-type center thermal annealing in heavy-ion and neutron irradiated Al_2O_3 single crystals. — Nucl. Instrum. Methods Phys. Res. B, 2018, **433**, pp. 93-97.

468. A. Gopejenko, Yu.A. Mastrikov, Yu.F. Zhukovskii, E.A. Kotomin, P.V. Vladimirov, and A. Moeslang. Ab initio modelling of the Y, O, and Ti solute interaction in fcc-Fe matrix. – Nucl. Instrum. Methods Phys. Res. B, 2018, **433**, pp. 106-110.

469. Yu. A. Mastrikov, R. Merkle, E. A. Kotomin, M. M. Kuklja, J. Maier. Surface termination effects on the oxygen reduction reaction rate at fuel cell cathodes. – J. Mater. Chem. A, 2018, **6**, pp. 11929.

470. M.F. Hoedl, E. Makagon, I. Lubomirsky, R. Merkle, E.A. Kotomin, and J. Maier. Impact of point defects on the elastic properties of $BaZrO_3$: comprehensive insight from experiments and ab initio calculations. — Acta Mater., 2018, **160**, pp. 247-256.

471. G.A. Kaptagay, Yu.A. Mastrikov, and E.A. Kotomin. First-principles modelling of N-doped Co_3O_4. — Latv. J. Phys. Tech. Sci., 2018, **55**, Nr 5, pp. 36-42

472. V.N. Kuzovkov, E.A. Kotomin, and A.I. Popov. Kinetics of dimer F_2 type center annealing in MgF_2 crystals. — Nucl. Instrum. Methods Phys. Res. B, 2018, **435**, pp. 7982

473. A. Platonenko, D. Gryaznov, Yu.F. Zhukovskii, and E.A. Kotomin. Ab initio simulations on charged interstitial oxygen migration in corundum. — Nucl. Instrum. Methods Phys. Res. B, 2018, **435**, pp. 7478.

474. Yu.A. Mastrikov, M.N. Sokolov, S. Koch, Yu.F. Zhukovskii, A. Gopejenko, P.V. Vladimirov, V.A. Borodin, E.A. Kotomin, and A. Mslang. Ab initio modelling of the

initial stages of the ODS particle formation process. — Nucl. Instrum. Methods Phys. Res. B, 2018, **435** , pp. 7073.

475. Yu.A. Mastrikov, M.N. Sokolov, E.A. Kotomin, A. Gopejenko, and Yu.F. Zhukovskii. Ab initio modeling of Y and O solute atom interaction in small clusters within the bcc iron lattice. – Phys. Status Solidi B, 2018, **255**, 187346 (pp. 1-5)

476. A. Platonenko, D. Gryaznov, Yu.F. Zhukovskii, and E.A. Kotomin. First principles simulations on migration paths of oxygen interstitials in MgAl2O4. — Phys. Status Solidi B, 2018, **255**, 1800282 (pp. 1-7).

477. D. Fuks, D. Gryaznov, E.A. Kotomin, A. Chesnokov, and J. Maier. Dopant solubility in ceria: alloy thermodynamics combined with the DFT+U calculations. — Solid State Ionics, 2018, **325**, pp. 258264

478. A.B. Usseinov, Yu.F. Zhukovskii, E.A. Kotomin, A.T. Akilbekov, M.V. Zdorovets, G.M. Baubekova, and Zh.T. Karipbayev. Transition levels of acceptor impurities in ZnO crystals by DFT-LCAO calculations. — J. Phys.: Conf. Ser., 2018, **1115**, 042064 (pp.1-7).

479. G.A. Kaptagay, Yu.A. Mastrikov, E.A. Kotomin, S.A. Sandibaeva, A.S. Kopenbaeva, G.O. Baitasheva, and L.S. Baikadamova. Theoretical investigations of nitrogen doping on Co3O4 for water dissociation catalytically activity. — J. Phys.: Conf. Ser., 2018, **1115**, 032032 (pp.1-6).

2019

480. L.L. Rusevich, G. Zvejnieks, E.A. Kotomin, M. Macek Krzmanc, A. Meden, S. Kunej, I.D. Vlaicu. Theoretical and experimental study of (Ba,Sr)TiO_3 perovskite solid solutions and BaTiO3 – SrTiO3 heterostructures. – J. Phys. Chem. C, 2019, **123**, pp. 2031-2036.

481. E. Heifets, E. A. Kotomin, A. A. Bagaturyants, J. Maier. Thermodynamic stability of non-stoichiometric $SrFeO_3$: a hybrid DFT study. – Chem. Phys. Phys. Chem. 2019, **21**, 3918.

482. A. Chesnokov, D. Gryaznov, E.A. Kotomin. First principles calculations on CeO_2 doped with Tb3+ ions. – Optical Materials, 2019, **90**, 76-83.

483. N. Sobolev, F. Djurabekova, E.A. Kotomin. Defect-induced effects in nanomaterials. — Phys. Status Solidi B, 2019, **256**, 1900181 (pp. 1-2)

484. Yu.A. Mastrikov, M.N. Sokolov, E.A. Kotomin, A. Gopejenko, Yu.F. Zhukovskii. Ab initio modeling of Y and O solute atom interaction in small clusters within the bcc iron lattice. – Phys. Status Solidi B, 2019, **256**, 1800346 (pp. 1-5)

485. A. Platonenko, D. Gryaznov, Yu.F. Zhukovskii, E.A. Kotomin. First principles simulations on migration paths of oxygen interstitials in MgAl2O4. – Phys. Status Solidi B, 2019, **256**, 1800282 (pp. 1-7).

486. L.L. Rusevich, G. Zvejnieks, E.A. Kotomin. Ab initio simulation of (Ba,Sr)TiO_3 and (Ba,Ca)TiO_3 perovskite solid solutions. – Solid State Ionics, 2019, **337**, pp. 7681.

487. R.A. Evarestov, A. Senocrate, E.A. Kotomin, J. Maier. First-principles calculations of iodine-related point defects in $CsPbI_3$. – Phys. Chem. Chem. Phys., 2019, **21**, pp. 7841-7846

488. D. Zablotsky, L.L. Rusevich, G. Zvejnieks, V. Kuzovkov, E. Kotomin. Manifestation of dipole-induced disorder in self-assembly of ferroelectric and ferromagnetic nanocubes. — Nanoscale, 2019, **11**, pp. 7293-7303.

489. A.B. Usseinov, A.T. Akilbekov, E.A. Kotomin, A.I. Popov, D.D. Seitov, K.A. Nekrasov, Sh.G. Giniyatova, Zh.T. Karipbayev. The first principles calculations of CO2 Adsorption on (10-10) ZnO surface. — AIP Conf. Proc., 2019, 2174, 020181 (pp. 1-6).

500. G. Zvejnieks, L.L. Rusevich, D. Gryaznov, E.A. Kotomin. Interface-induced enhancement of piezoelectricity in the (SrTiO3)m–(BaTiO3)M-m superlattice for energy harvesting applications. — Phys. Chem. Chem. Phys., 2019, 21, pp. 23541-23551.

501. A. Platonenko, F.S. Gentile, J. Maul, F. Pascale, E.A. Kotomin, R. Dovesi. Nitrogen interstitial defects in silicon. A quantum mechanical investigation of the structural, electronic and vibrational properties.— Mater. Today Commun., 2019, **21**, 100616 (pp. 1-13).

2020

502. G. Baubekova, A. Akilbekov, E.A. Kotomin, V.N. Kuzovkov, A.I. Popov, E. Shablonin, E. Vasil'chenko, M. Zdorovets, A. Lushchik. Thermal annealing of radiation damage produced by swift Xe132 ions in MgO single crystals. — Nucl. Instrum. Methods Phys. Res. B, 2020, **462**, pp. 163168.

503. E. A. Kotomin, Yu.A. Mastrikov, R. Merkle, J. Maier. First principles calculations of oxygen reduction reaction at fuel cell cathodes. – Current Opinion in Electrochemistry, 2020, **19**,122128

504. T.S. Bjoerheim, M.F. Hoedl, R. Merkle, E.A. Kotomin, J. Maier. Proton, hydroxide ion, and oxide ion affinities of closed-shell oxides: Importance for the hydration reaction and correlation to electronic structure. – J. Phys. Chem. C, 2020, **124**, pp. 1277-1284.

505. A.U. Abuova, Yu.A. Mastrikov, E.A. Kotomin, S.N. Piskunov, T.M. Inerbaev, A.T. Akilbekov. First-principles modeling of oxygen adsorption on Ag-doped LaMnO3 (001) surface. – J. Electron. Mater., 2020, **49**, pp. 14211434.

506. A. Platonenko, D. Gryaznov, E.A. Kotomin, A. Lushchik, V. Seeman, A.I.Popov. Hybrid functional calculations of hyperfine coupling tensor for hole-type defects in MgAlO4. – Nucl.Inst.Methods Phys. Res. B, 2020, **464**, pp. 60-64.

507. M.F. Hoedl, D. Gryaznov, R. Merkle, E.A. Kotomin, J. Maier. Interdependence of oxygenation and hydration in mixed-conducting (Ba,Sr)FeO(3) perovskites studied by density functional theory. — J. Phys. Chem. C, 2020, **124**, pp. 1178011789.

508. D. Gryaznov, S.K. Stauffer, E.A. Kotomin, L. Vilciauskas. Hybrid density functional theoretical study of NASICON-type NaxTi2(PO4)3 (x = 14). — Phys. Chem. Chem. Phys., 2020, **22**, pp. 11861-11870.

509. N.V. Krainyukova, V.O. Hamalii, A.V. Peschanskii, .. Popov, E.A. Kotomin. Low temperature structural transformations on the (001) surface of SrTiO3 single crystals. — Low Temp. Phys., 2020, **46**, pp. 740-750.

510. A. Lushchik, E. Feldbach, E.A. Kotomin, I. Kudryavtseva, V.N . Kuzovkov, A.I . Popov, V. Seeman, E. Shablonin. Distinctive features of diffusion-controlled radiation defect recombination in stoichiometric magnesium aluminate spinel single crystals and transparent polycrystalline ceramics. —- Sci. Rep., 2020, **10**, 7810 (pp. 1-9).

511. R.A. Evarestov, E.A. Kotomin, A. Senocrate, R.K. Kremer, J. Maier. First-principles comparative study of perfect and defective CsPbX3 (X = Br, I) crystals. — Phys. Chem. Chem. Phys., 2020, **22**, pp. 3914-3920.

512. D. Zablotsky, V.N. Kuzovkov, E.A. Kotomin. Role of intrinsic dipoles in the evaporation-driven assembly of perovskite nanocubes into energy-harvesting composites. — Phys. Status Solidi A, 2020, **217**, 1900533 (pp. 1-6).

513. A.B. Usseinov, D. Gryaznov, A.I. Popov, E.A. Kotomin, D. Seitov, F. Abuova, K.A. Nekrasov, A.T. Akilbekov. Ab initio calculations of pure and Co+2-doped MgF2 crystals. — Nucl. Instrum. Methods Phys. Res. B, 2020, **470**, pp. 1014.

514. A. Senocrate, E. Kotomin, J. Maier. On the way to optoionics. – Helvetica Chimica Acta, 2020, **103**, e2000073 (pp. 1-8).

515. A.I. Popov, E. Elsts, E.A. Kotomin, A. Moskina, Z.T. Karipbayev, I. Makarenko, S. Pazylbek, V.N. Kuzovkov. Thermal annealing of radiation defects in MgF2 single crystals induced by neutrons at low temperatures. — Nucl. Instrum. Methods Phys. Res. B, 2020, **480**, pp. 1621.

516. V.N. Kuzovkov, E.A. Kotomin, A.I. Popov, R. Vila. Peculiarities of the diffusion-controlled radiation defect accumulation kinetics under high fluencies. – Nucl. Instrum. Methods Phys. Res. B, 2020, **480**, pp. 4548.

517. L.L. Rusevich, E.A. Kotomin, G. Zvejnieks, A.I. Popov. Ab initio calculations of structural, electronic and vibrational properties of BaTiO3 and SrTiO3 perovskite crystals with oxygen vacancies. — Low Temp. Phys., 2020, **46**, pp. 11851195.

518. M.N. Sokolov, Yu.A. Mastrikov, A. Gopejenko, D. Bocharov, Yu.F. Zhukovskii, E.A. Kotomin. Ab initio modelling of titanium impurities in -Fe lattice. — Nucl. Instrum. Methods Phys. Res. B, 2020, **483**, pp. 50-54.

519. A. Platonenko, D. Gryaznov, A.I. Popov, R. Dovesi, E.A. Kotomin. First principles calculations of the vibrational properties of single and dimer F-type centers in corundum crystals. — J. Chem. Phys., 2020, **153**, 134107 (pp. 1-9).

520. V. Seeman, A. Lushchik, E. Shablonin, G. Prieditis, D. Gryaznov, A. Platonenko, E.A. Kotomin, A.I. Popov. Atomic, electronic and magnetic structure of an oxygen interstitial in neutron irradiated Al2O3 single crystals. — Sci. Rep., 2020, **10**, 15852 (pp. 1-14).

2021

521. M.Ya. Rudysh, P.A. Shchepanskyi, A.O. Fedorchuk, M.G. Brik, V.Yo. Stadnyk, G.L. Myronchuk, E.A. Kotomin, M. Piasecki. Impact of anionic system modification on the desired properties for CuGa(S1-xSex)2 solid solutions. — Comput. Mater. Sci., 2021, **196**, 110553 (pp. 1-10)

522. A. Chesnokov, D. Gryaznov, N.V. Skorodumova, E.A. Kotomin, A. Zitolo, M. Zubkins, A. Kuzmin, A. Anspoks, J. Purans. The local atomic structure and thermoelectric properties of Ir-doped ZnO: hybrid DFT calculations and XAS experiments. — J. Mater. Chem. C, 2021, **9**, pp. 49484960

523. V. Serga, R. Burve, A. Krumina, M. Romanova, E.A. Kotomin, A.I. Popov. Extractionpyrolytic method for TiO2 polymorphs production. — MDPI Crystals, 2021, **11**, 431 (pp. 1-13)

524. M. Tyunina, L.L. Rusevich, E.A. Kotomin, O. Pacherova, T. Kocourek, A. Dejneka. Epitaxial growth of perovskite oxide films facilitated by oxygen vacancies. — J. Mater. Chem. C, 2021, **9**, pp. 1693-1700

525. G. Zvejnieks, D. Zavickis, E.A. Kotomin, D. Gryaznov. $BaCoO_3$ monoclinic structure and chemical bonding analysis: hybrid DFT calculations. — Phys. Chem. Chem. Phys., 2021, **23**, pp. 1749317501.

526. Yu.A. Mastrikov, N.G. Chuklina, M.N. Sokolov, A.I. Popov, D.V. Gryaznov, E.A. Kotomin, J. Maier. Small radius electron and hole polarons in PbX_2 (X = F, Cl, Br) crystals: a computational study. — J. Mater. Chem. C, 2021,**9**, 16536 (pp. 1-9)

527. M. Sokolov, Yu.A. Mastrikov, G. Zvejnieks, D. Bocharov, E.A. Kotomin, V. Krasnenko. Water splitting on multifaceted SrTiO3 nanocrystals: computational study. — MDPI Catalysts, 2021, **11**, 1326 (pp. 1-8).

528. L.L. Rusevich, M. Tyunina, E.A. Kotomin, N. Nepomniashchaia, A. Dejneka. The electronic properties of SrTiO3 with oxygen vacancies or substitutions. – Sci. Rep., 2021, **11**, 23341 (pp. 1-8).

529. A. Lushchik, V.N. Kuzovkov, E.A. Kotomin, G. Prieditis, V. Seeman, E. Shablonin, E. Vasilchenko, A.I. Popov. Evidence for the formation of two types of oxygen interstitials in neutronirradiated aAl2O3 single crystals. —Sci. Rep., 2021, **11**, 20909 (pp. 1-10).

2022

530. R.I. Eglitis, E.A. Kotomin, A.I. Popov, S.P. Kruchinin, R. Jia. Comparative ab initio calculations of SrTiO3, BaTiO3, PbTiO3, and SrZrO3 (001) and (111) surfaces as well as oxygen vacancies. — Fiz. Nizk. Temp. 2022, **48**, pp. 8796.

531. L.L. Rusevich, E.A. Kotomin, A.I. Popov, G. Aiello, T.A. Scherer, A. Lushchik. The vibrational and dielectric properties of diamond with N impurities: First principles study. – Diamond and Relat. Mater., 2022, **130**, 109399 (pp. 1-7).

532. Yu.A. Mastrikov, D. Gryaznov, G. Zvejnieks, M.N. Sokolov, M. Putnia, E.A. Kotomin. Sr doping and oxygen vacancy formation in La1-xSrxScO3- solid solutions: Computational modelling. – MDPI Crystals, 2022, **12**, 1300 (pp. 1-17). Open Access.

533. V. Krasnenko, L.L. Rusevich, A. Platonenko, Yu.A. Mastrikov, M. Sokolov, E.A. Kotomin. Water splitting on multifaceted SrTiO3 nanocrystals: calculations of Raman vibrational spectrum. — MDPI Materials, 2022, **15**, 4233 (pp. 1-17). Open Access.

534. A. Lushchik, V. Seeman, E. Shablonin, E. Vasilchenko, V.N. Kuzovkov, E.A. Kotomin, A.I. Popov. Detection of hidden oxygen interstitials in neutron-irradiated corundum crystals. — Optical Materials X, 2022, **14**, 100151 (pp. 1-10). Open Access.

535. Yu.A. Mastrikov, D. Gryaznov, M.N. Sokolov, G. Zvejnieks, A.I. Popov, R.I. Eglitis, E.A. Kotomin, M.V. Ananyev. Oxygen vacancy formation and migration within the antiphase boundaries in lanthanum scandate-based oxides: computational study. — MDPI Materials, 2022, **15**, 2695 (pp. 1-10). Open Access.

536. Y.-R. Wang, G.Y. Kim, E. Kotomin, D. Moia, J. Maier. Photo de-mixing in mixed halide perovskites: the roles of ions and electrons. — J. Phys. Energy, 2022, **4**, 011001 (pp. 1-11). Open Access.

537. Y.-P. Lin, D. Bocharov, E.A. Kotomin, M.G. Brik, S. Piskunov. Influence of Au, Ag, and Cu adatoms on optical properties of TiO2 (110) surface: predictions from RT-TDDFT calculations. — MDPI Crystals, 2022, **12**, 452 (pp. 1-14). Open Access.

538. R.I. Eglitis, E.A. Kotomin, A.I. Popov, S.P. Kruchinin, R. Jia Comparative ab initio calculations of SrTiO3, BaTiO3, PbTiO3, and SrZrO3 (001) and (111) surfaces as well as oxygen vacancies. — Low Temp. Phys., 2022, **48**, pp. 80-88.

539. A. Lushchik, V.N. Kuzovkov, I. Kudryavtseva, A.I. Popov, V. Seeman, E. Shablonin, E. Vasilchenko, E.A. Kotomin. The two types of oxygen interstitials in neutron-irradiated corundum single crystals: joint experimental and theoretical study. Phys. Status Solidi B, 2022, **259**, 2100317 (pp. 1-7).

540. E.A. Kotomin, A. Kuzmin, Ju. Purans, Ja. Timoshenko, S. Piskunov, R. Merkle, J. Maier. Theoretical and experimental studies of charge ordering in CaFeO3 and SrFeO3 crystals. — Phys. Status Solidi B, 2021, **259**, 2100238 (pp. 1-6).

541. L.L. Rusevich, E.A. Kotomin, G. Zvejnieks, M. Macek Krzmanc, S. Gupta, N. Daneu, J.C.S. Wu, Y.-G. Lee, W.-Y. Yu. Effects of Al doping on hydrogen production efficiency upon photostimulated water splitting on SrTiO3 nanoparticles. J. Phys. Chem. C, 2022, **126**, pp. 2122321233

2023

542. V. Kuzovkov, E. A. Kotomin, R. Vila. Theoretical analysis of thermal annealing kinetics of radiation defects in silica. J. Nucl. Mater., 2023, **579**, 154381 (pp. 1-5).

543. M. Sokolov, Yu.A. Mastrikov, G. Zvejnieks, D. Bocharov, V. Krasnenko, K.S. Exner, E.A. Kotomin. First principles calculations of hydrogen evolution reaction and proton migration on stepped surfaces of SrTiO3. Adv. Theory Simul., 2023, xxx, 2200619 (pp. 1-7). Open Access

544. N.V. Krainyukova, V.O. Hamalii, L.L. Rusevich, E.A. Kotomin, J. Maier. Effect of 'in-plane' contraction on the (001) surface of the model perovskite SrTiO3. Appl. Surf. Sci., 2023, **615**, 156297 (pp. 1-7).

545. Y.-Y. Tai, J.C.S. Wu, W.-Y. Yu, M. Maek Krmanc*, E.A. Kotomin. Photocatalytic water splitting of improved strontium titanate for simultaneous separation of H2 in a twin photoreactor. Appl. Catal. B, 2023, **324**, 122183 (pp. 1-10).

546. M.F. Hoedl, A. Chesnokov, D. Gryaznov, R. Merkle, E.A. Kotomin, J. Maier. Proton migration barriers in BaFeO3 insights from DFT calculations. J. Mater. Chem. A, 2023, **11** , pp. 6336-6348. Open Access

547. Y.-G. Lee, Y.-C. Cheng, Y.-T. Lin, J.C.S. Wu, W.-Y. Yu, M. Macek Krzmanc, S. Gupta, E.A. Kotomin. Photocatalytic water splitting of Al-doped RhxCr2xO3/SrTiO3 synthesized by flux method: Elucidating the role of different molten salts.— J. Phys. Chem. C, 2023, **127**, pp. 99819991.

548. V. Krasnenko, A. Platonenko, A. Liivand, L.L. Rusevich, Yu.A. Mastrikov, G. Zvejnieks, M. Sokolov, E.A. Kotomin. Modeling of the lattice dynamics in strontium titanate films of various thicknesses: Raman scattering studies. Materials, 2023, **16**, 6207 (pp. 1-15)

549. M. Tyunina, L.L. Rusevich, M. Savinov, E.A. Kotomin, A. Dejneka. Dielectric behaviour of nitrogen doped perovskite SrTiO3-N films. — J. Mater. Chem. C, 2023, **11** , pp. 1668916698.

2024

550. A. Platonenko, V. Pankratov, E.A. Kotomin, A. Dauletbekova, A.I. Popov. Ab initio study on the vibrational and electronic properties of radiation-induced defects in potassium bromide. Crystals 2024, **14**, 161 (pp. 1-11).

551. N.V. Krainyukova, D.G. Diachenko, E.A. Kotomin. Selective uptake and desorption of carbon dioxide in carbon honeycombs of different sizes. — Low Temp. Phys. 2024, **50**, 97102.

552. N.V. Krainyukova, D.G. Diachenko, E.A. Kotomin. Selective uptake and desorption of carbon dioxide in carbon honeycombs of different sizes. — Fiz. Nizk. Temp. / Low Temp. Phys. 2024, **50**, 102107.

553. V.N. Kuzovkov, E.A. Kotomin, A. Lushchik, A.I. Popov, E. Shablonin. The annealing kinetics of the F-type defects in MgAl2O4 spinel single crystals irradiated by swift heavy ions. – Opt. Mater. 2024, **147**, 114733 (pp. 1-6).

554. G. Zvejnieks, L.L. Rusevich, E. Heifets, E.A. Kotomin, D. Gryaznov. A visual representation for accurate local basis set construction and optimization: A case study of SrTiO3 with hybrid DFT functionals. —- Crystals 2024, **14**, 671 (pp. 1-18).

555. E.A. Kotomin, V.N. Kuzovkov, A. Lushchik, A.I. Popov, E. Shablonin, T. Scherer, E. Vasilchenko. The annealing kinetics of defects in CVD diamond irradiated by Xe ions. — Crystals 2024, **14**, 546 (pp. 1-14).

556. T.M. Inerbaev, A.U. Abuova, Zh.Ye. Zakiyeva, F.U. Abuova, Yu.A. Mastrikov, M. Sokolov, D. Gryaznov, E.A. Kotomin. Effect of Rh doping on optical absorption and oxygen evolution reaction activity on BaTiO3 (001) surfaces. — Molecules 2024, **29**, 2707 (pp. 1-15).

557. L.L. Rusevich, E.A. Kotomin, A.I. Popov, G. Aiello, T.A. Scherer, A. Lushchik. The electronic, vibrational and dielectric properties of diamond crystals with neutral vacancies: first principles study. Opt. Mater. 2024, **150**, 115222 (pp. 1-9).

558. M. Sokolov, Yu.A. Mastrikov, D. Bocharov, V. Krasnenko, G. Zvejnieks, K.S. Exner, E.A. Kotomin. Computational study of oxygen evolution reaction on flat and stepped surfaces of strontium titanate. —- Catal. Today 2024, **432**, 114609 (pp. 1-7).

559. Y.-P. Lin, E. Neilande, H. Bandarenka, S. Zavatski, I. Isakovica, S. Piskunov, D. Bocharov, E.A. Kotomin. Excited state calculations of Cu-doped anatase TiO2 (101) and (001) nanofilms. — Crystals 2024, **14**, 247 (pp. 1-16).

560. L.L. Rusevich, M.G. Brik, D. Gryaznov, A.M. Srivastava, I. Chervyakov, G. Zvejnieks, D. Bocharov, E.A. Kotomin. First-principles linear combination of atomic orbitals calculations of K2SiF6 crystal: structural, electronic, elastic, vibrational and dielectric properties. — Materials 2024, **17**, 4865 (pp. 1-17)

2025

561. A. Chesnokov, D. Gryaznov, E.A. Kotomin, J. Maier, R. Merkle. Protons in (Ga,Sc,In,Y) 3+ doped BaFeO3 triple conductors Site energies and migration barriers investigated by density functional theory calculations. – Solid state ionics, 2025, **421**, 116788. Open Access.

562. A. Lushchik, A. Podelinska, V. Seeman, E. Shablonin, E. A. Kotomin, and V. N. Kuzovkov. Open Questions on the Thermal Stability of Primary Electronic Centers in Irradiated MgO Single Crystals. – J. Phys. Chem. C, 2025, **129**, 27752781

563. R. Merkle, M.F. Hoedl, A. Chesnokov, D. Gryaznov, E. Bucher, E.A. Kotomin, W. Sitte, J. Maier. Electronic structure, phase formation, and defect distribution in the Ba(Ce,Fe,Acc)O3- system. Acta Mater, 2025, **287**, 120739. Open Access

564. I. Mihailovs, E. Belobrovko, A. Bundulis, D.V. Bocharov, E.A. Kotomin, M. Rutkis. Use of factorial design for calculation of second hyperpolarizabilities. Nanomaterials 2025, **15**, 1302. Open Access

565. E.A. Kotomin, R. Assylbayev, G. Baubekova, I. Kudryavtseva, V.N. Kuzovkov, A. Podelinska, V. Seeman, E. Shablonin, A. Lushchik. Annealing of oxygen-related Frenkel defects in corundum single crystals irradiated with energetic xenon ions. Crystals 2025, **15**, 573. Open Access.

566. L.L. Rusevich, M.G. Brik, D. Gryaznov, A.M. Srivastava, I.D. Chervyakov, G. Zvejnieks, D. Bocharov, E.A. Kotomin. A comparative study of A2SiF6 (A = Cs, K) phosphor host matrices: Linear combination of atomic orbital hybrid density functional theory calculations. Materials 2025, **18**, 2025. Open Access

577. M. Tyunina, L.L. Rusevich, M. Savinov, T. Kocourek, O. Pacherova, A. Dejneka, E.A. Kotomin. Substrate-controlled response coefficients in thin films. Adv. Sci. 2025, **12**, e05761.

578. M.A. Kabanenko, V.O. Hamalii, D.G. Diachenko, Y.A. Mastrikov, E.A.Kotomin, N.V. Krainyukova. Pseudophysical sorption of aluminum in carbon honeycomb structures. Low Temp. Phys. 2025, **51**, 11981204.

579. Yu.A. Mastrikov, D. Gryaznov, A. Chesnokov, G. Zvejnieks, M. Sokolov, M.M. Kuklja, R. Merkle, E.A. Kotomin. Oxygen defect formation and migration in Sr2FeO4: Insights from first principles DFT calculations with the PBE+U functional. Phys. Rev. Mater. 2025, **9**, 105801

580. I. Mihailovs, E. Belobrovko, A. Bundulis, D.V. Bocharov, E.A. Kotomin, M. Rutkis. Use of factorial design for calculation of second hyperpolarizabilities. Nanomaterials 2025, **15**, 1302.

2026

581. M. Tyunina, L.L. Rusevich, E. de Prado, N. Nepomniashchaia, T. Kocourek, A.E. Kotomin, A. Dejneka. Electronic structure modulation via Mn(Ti) doping in epitaxial SrTi1-xMnxO3. Mater. Adv. 2026, **7**, 87728781.

582. Yu.A. Mastrikov, D. Gryaznov, A. Chesnokov, G. Zvejnieks, M. Sokolov, M.M. Kuklja, R. Merkle, E. Kotomin. First-principles study of Sr2xLaxFeO4 and comparison with Sr2FeO4: The nature of the positively charged defect determines the character of the electronic structure. J. Phys. Chem. C 2026, **130**, 1100111008.

583. V. Hamalii, M. Kabanenko, D. Diachenko, Yu. Mastrikov, E. Kotomin, N. Krainyukova. Selective argon uptake and structural ordering in carbon honeycomb nanostructures. Int. J. Mol. Sci. 2026, **27**, 6410

584. Zh.Ye. Zakiyeva, U.Zh. Tolegen, T.M. Inerbaev, E.A. Kotomin, A.U. Abuova, B. Akilbekov, A. Amankeldiyeva, A. Zhomartova, A.I. Popov, O.K. Abdirashev, F.U. Abuova. Atomic-scale understanding of doping effects in BaTiO3 in the presence of water: Implications for photocatalytic water splitting. Materials 2026, **19**, 2336.

585. Yen-Po Liu, M. Weber, D. Jennings, L. Rusevich, E.Kotomin, R.Timm, F. Gunkel, R.Dittmann. Partial Phase Separation in the Growth Mode of Exsolution Active SrTiN-iNbO3 Thin Films. Advanced Science, 2026, 0:e76812.

Abstracts

A-1. Evarestov R.A., Ermoshkin A.N., Kotomin E.A. Use of the molecular cluster model for calculating impurities and defects in MgO crystal. -In: 3. Sov. conf. on physics and chemistry of ionic solids. Abstracts. Inst. of phys., Latv. Acad.Sci, 1975, p.119.

A-2. Ermoshkin A.N., Evarestov R.A., Kotomin E.A. Molecular models of point defects in MgO crystal. -In: 8. Ural Conf. on Spectroscopy. Abstracts. Sverdlovsk: Ural Polyt. Inst., 1975, p.18.

A-3. Kotomin E.A., Tale I.A. Models of the temperature dependence of the efficiency of Frenkel defect accumulation in ionic crystals. -In: 23. Sov. conf. on Luminescence. Abstracts. Kishinev State Univ. press, 1976, p.71.

A-4. Kotomin E.A., Tale I.A., Fabrikant I.I. Two models for temperature dependence of F centre accumulation efficiency in doped alkali halides. -In: Int.Conf. on Defects in Insulating Crystals. Abstracts. Gatliburg, USA, 1977. P.247-248.

A-5. Kotomin E.A., Valdats G.A. Computer simulation of low-tempe- rature accumulation of F and H centres. -In: Sov.sem. on radiation defect computer simulations. Abstracts. Kr.Rog pedagog. Inst., 1977, p.41-43.

A-6. Kotomin E.A. Accumulation of radiation defects in insulators limited by tunnelling recombination. -Sov.Symp. on radiation chemistry. Abstracts. Tbilisi, 1978, p.193-194.

A-7. Kotomin E.A. Theory of diffusion-controlled tunnelling recombination of defects in liquids and solids. -Sov. Symp. on Rad. Chem. Abstracts. Tbilisi, Inst.phys., 1978, p.195.

A-8. Shluger A.L., Kotomin E.A. Quantum chemical estimates of the tunnelling recombination probability of close $F-H$ centres. -In: Sov.conf. on physics and chemistry of ionic crystals. Abstracts. Inst. of phys., Latv.Aca.Sci., 1978, p.345-346.

A-9. Kotomin E.A., Fabrikant I.I. Influence of the elastic interaction with in Frenkel pairs upon their accumulation in crystals. -In: Sov.conf. on physics and chemistry of ionic crystals. Abstracts. Inst. of phys., Latv.Aca.Sci., 1978, p.61-62.

A-10. Kotomin E.A., Fabrikant I.I. Theory of diffusion-controlled tunnelling recombination of defects. -In: Sov.symp. on Quant.Chem. Abstracts. Novosibirsk, Inst. of Chem. Kinetics of the Aca. of Sci.of the USSR, 1978, p.115.

A-11. Kotomin E.A., Tale I.A. Kinetics of the diffusion-controlled tunnelling recombination of V_k centres in alkali halides. -In: XYII Sov.Conf. on Lumin., Ezernieki: Latv. Univ. Press, 1980, p.74.

A-12. Kotomin E.A., Shluger A.L. Tunnelling recombination of the electronic and hole centres in alkali halides. -In: Sov.sem. on radiation defect computer simulations. Abstracts. Lielupe, Inst. phys., Latv. Aca. Sci., 1980, p.26.

A-13. Kotomin E.A., Kuzovkov V.N. Radiation-induced defect clustering in crystals. -In: Sov.sem. on rad. defect computer simulations. Abstracts. Lielupe, Inst. phys., Latv. Aca. Sci., 1980, p.27.

A-14. Kotomin E.A., Kuzovkov V.N. Generalized kinetics of diffusion-controlled recombination of defects in crystals. -In: 42. Sov. conf. on Lumin. Abstracts. Ezernieki: Latv.Univ. press, 1980, p.60.

A-15. Kotomin E.A., Nagornyi A.N., Tale I.A., Tale V.G. Impurity hopping recombination in mixed and heavily-doped alkali halide crystals. -In: Intern. Conf. on Defects in Insulators. Abstracts. Riga, 1981, P.285.

A-16. Kotomin E.A., Shluger A.L., Kantorovich L.N., Tale I.A. Tunnelling recombination and electron impurity hopping in KCl crystal. -In: 1. Sov. Conf. on Quant. Chem. of Solids. Leningrad Univ. press. Abstracts. 1982, p.78-79.

A-17. Shluger A.L., Kotomin E.A., Dzelme Yu.R. Electronic sructure of point defects near LiF surface. -In: 1.Sov.Conf. on Quant. Chem. of Solids. Leningrad Univ.press. Abstracts. 1982, p.85-86.

A-18. Kotomin E.A., Shluger A.L. Modification of the INDO method for calculating defects in ionic crystals. -In: Sov.Conf. on Quant. Chem. of Solids. Leningrad Univ.press. Abstracts. 1982, p.78-79.

A-19. Kuzovkov V.N., Kotomin E.A. Kinetics of the diffusion- controlled $A + B \to B$ reaction. -In: 1.Sov.Conf. on Quant. Chem. of Solids. Leningrad Univ.press. Abstracts. 1982, p.117.

A-20. Shluger A.L., Kotomin E.A. Theory of the electronic structure of perfect ionic crystal surfaces -In: 3. Sov. symp. on Ioniz. Rad. Imp. on heter.syst. Abstracts. Kemerovo St.Univ. 1982, p.70.

A-21. Dzelme Yu.R., Kotomin E.A., Shluger A.L. Structure and tunnelling recombination of radiation defects in the bulk and on the surface of alkali halide crystals. -In: 3. Sov. symp. on Ioniz. Rad. Imp. on heter. syst. Abstracts. Kemerovo St.Univ., 1982, p.72.

A-22. Kotomin E.A., Shluger A.L. Quantum-chemical investigations of reactions between defects in ionic crystals. -In: Intern. Sem. on Quantum Chemistry. Abstracts. Libice, Czechosl., 1983. P.50.

A-23. Kotomin E.A., Kuzovkov V.N., Tale I.A. Many-particle effects in accumulation kinetics of immobile Frenkel defects in crystals. -In: 5.Sov.Conf. on phys. and chem. of ionic crystals. Abstracts. Inst. of phys., Latv.Aca.Sci., 1983, p.160.

A-24. Kotomin E.A., Shluger A.L. Use of molecular models in calculating the radiation defect structure in MgO, SiO_2 and Li_2SiO_3. -In: 5.Sov.Conf. on phys. and chem. of ionic crystals. Abstracts. Inst. of phys., Latv.Aca.Sci., 1983, p.92-94.

A-25. Shluger A.L., Kotomin E.A., Kantorovich L.N., Tale I.A. Calculations of radiation defect structure in oxide crystals. -Sov.Conf. on Rad. Physics of semic. and related. comp. Abstracts. Tashkent, 1984, p.194.

A-26. Kotomin E.A., Shluger A.L. Theoretical simulations of reactions in non-metallic crystals with defects. -In: 2. Sov. Conf. on Quant. Chem. of Solids. Abstracts. Riga: Latv.Univ., 1985, p.31-32.

A-27. Kotomin E.A., Tale I.A., Tale V.G., Butlers P.I. Kinetics of the non-steady diffusion-controlled tunnelling recombination of defects in solids. -In: 2. Sov. Conf. on Quant. Chem. of Solids. Abstracts. Riga: Latv.Univ., 1985, p.46.

A-28. Shluger A.L., Kotomin E.A., Zakis Yu.R. Quantum chemical simulation of the electronic and spatial structure of intrinsic defects in silicates. -In: 8.Sov.symp. on the glassy state. Abstracts. Leningrad, 1986, p.440-441.

A-29. Kotomin E., Tale I., Tale V., Butlers P., Kulis P. Non-steady- state diffusion-controlled tunnelling recombination of defects. -In: Intern. Conf. on Defects in Insulating Crystals. Abstracts. Parma, 1988. P.50.

A-30. Kotomin E., Kinetics of non-steady-state recombination processes in solids controlled by defect hopping and electron tunnelling. -In: Emil Warburg Symposium on Dynamical Processes in Condensed Molecular Systems. Abstracts. Bayreuth, Germany, 1990. P.21.

A-31. Kotomin E.A., Stefanovich E.V., Stashans A., Tale I.A. Semiempirical simulation of hole self-trapping in corundum. -In: Conf. on Quantum Chemistry of Solids. Abstracts. Riga. 1990. P.204-205.

A-32. Kotomin E.A., Tale I.A. Kinetics of non-steady-state diffusion-controlled tunnelling recombination of defects in insulating solids. - In: Conf. on Quantum Chemistry of Solids. Abstracts. Riga. 1990. P.300

A-33. Millers D.K., Kotomin E.A., Grigorjeva L.G. Luminescence of mixed silver halides under powerful excitation. - Mater. Res. Soc. Meeting. Abstr. Boston, 1991. P.301.

A-34. Kotomin E., Popov A., Eglitis R. Kinetics of correlated annealing of radiation Frenkel defects in ionic crystals. -Conf. on Quantum Chemistry of Solids. Abstracts. Riga. 1990. P.135.

A-35. Kotomin E.A. The role of tunneling recombination in Frenkel defect recombination. In: 12 Conf. of Eur. Phys. Soc. Prague, 1992. Abstracts. P.300.

A-36. Kotomin E.A., Eglitis R., Popov A. Kinetics of correlated diffusion- controlled annealing of Frenkel defects in alkali halide crystals. - -Intern. Conf. on Defects in Insulating Materials. Abstracts (Nordkirchen, 1992). P.277.

A-37. Millers D.K., Grigorjeva L.G., Kotomin E. Intrinsic luminescence of mixed silver halides under powerful excitation as a probe of solid solution composition. -Ibid, p.392.

A-38. Kotomin E.A., Kuzovkov V.N. Cooperative phenomena in bimolecular reactions in solids with point defects. - Ibid., p.276.

A-39. Jacobs P.W.M., Kotomin E.A. Calculations of oxygen vacancy hopping in $\alpha - Al_2O_3$ crystal. - Ibid., p.22.

A-40. Jacobs P.W.M., Kotomin E.A., Stashans A., Tale I., Stefanovich E. Computer simulations of hole self-trapping in $\alpha - Al_2O_3$ crystal. - Ibid., p.144.

A-41. Kotomin E.A., Kuzovkov V.N. Many-particle effects in the kinetics of bimolecular reactions. - 18th IUPAP Int. Conf. on Statistical Physics. Abstracts. Berlin, 1992. P.360.

A-42. Kotomin E. Role of electron tunnelling in the kinetics of bimolecular processes in insulating solids with point defects. - Ibid., P.179.

A-43. Grigorjeva L.G.,Millers D.K., Kotomin E.A. Optical properties of IR fibers extruded from mixed silver halides. - OE/SPIE 92, Technical Conference 1792-22 on Components for Fiber Optics Appl.(Boston, 1992). Abstracts. P.312.

A-44. Kotomin E.A., Kuzovkov V.N. Cooperative phenomena in kinetics of bimolecular recombination of particles with Coulomb interaction. - Fall MRS Conf., Symposium **P** (Boston, 1992). Abstracts, p.519.

A-45. Kuzovkov V.N., Kotomin E.A. A novel many-point density formalism for the treatment of self-organization in reaction processes. - Ibid, p.522.

A-46. Jacobs P.W.M., Kotomin E.A. Modelling of Point Defects in Corundum Crystals. - Ibid., Symposium **O**, p.484.

A-47. Kuzovkov V.N., Kotomin E.A. The Kinetics of Defect Accumulation with Many-Particle Effects.- Abstr. Int. Conf. on Rad. Eff. in Insulators, Nagoya,1993, p. 121.

A-48. Kotomin E.A., Eglitis R.I., and Popov A.I. The Kinetics of Diffusion- Controlled Annihilation of Frenkel Defects in Alkali Halide Crystals, Ibid. p. 120.

A-49. Soppe W.J., Kotomin E.A.,and Zaiser M. Aggregation of Defects Under Irradiation: A Mesoscopic Approach. - Ibid., p.119.

A-50. Kotomin E.A. and Jacobs P.W.M. Theoretical Simulations of the Radiation-Induced Defect Properties in Insulating Materials. - Ibid.,p.11

A-51. Kotomin E.A., Tale I.A., Jacobs P.W.M., and Stashans A. Quantum Chemical Simulations of the Self-Trapped Hole Structure and Migration in Corundum Crystals. - Abstr. Int. Conf. on Luminescence, Storrs, 1993, p.Th5-71.

A-52. Kotomin E.A., Grigorjeva L., and Millers D.K. A Novel Model of Diffusion- Controlled Recombination Luminescence of Mixed Silver Halides. - Ibid, p. M5-89.

A-53. Kotomin E.A. and Popov A.I. Computer Simulations of I-Centre Annealing and Their Role in Low-Temperature TSL in Alkali Halides. - Ibid., p.M4-92.

A-54. Kotomin E.A., Millers D.K., Grigorjeva L.G., and Eglitis R.I. The Kinetics of Excitonic Luminescence in Mixed Silver Halides. - Abstr.MRS Meeting,1994, San Francisco, Symposium P, p. 328-329.

A-55. Kotomin E.A. Theory of Diffusion-Controlled Processes in Ionic Solids.- Ibid.,Symposium W, p. 474.

A-56. Kotomin E.A., Kuzovkov V.N., Zaiser M., and Soppe W. Diffusion- Controlled Defect Aggregation under Irradiation.- Ibid., Symposium W, p. 461.

A-57. Kotomin E.A., Kuzovkov V.N., Frank W., and Seeger A. Self-Organization Phenomena in the Bimolecular Annihilation Kinetics by Many-Particle Effects. - Ibid., p. 460.

A-58. Eglitis R., Kotomin E.A., and Popov A.I. Theoretical Simulations of I-Center Annealing in KCl and KBr Crystals. - Abstr. Eurodim- 94 Conf., Lyon, 1994, p.88.

A-59. Kotomin E.A., Stashans A.,and Jacobs P.W.M. Modelling of Point Defects in $\alpha - Al_2O_3$.- Ibid, p.89.

A-60. Kotomin E.A., Kuzovkov V.N., Zaiser M., and Soppe W. Theory of Diffusion-Controlled Defect Aggregation Under Irradiation: A Comparative Study of Three Basic Approaches. - Ibid, p.135.

A-61. Kotomin E.A., Popov A.I., and Hirai M. The Recombination Kinetics of Frenkel Defects in Alkali Halides: Contradiction between Pulsed and Steady-State Studies. - Ibid.,p.413.

A-62. Eglitis R., Kotomin E.A., Millers D.K., and Grigorjeva L.G.. Computer Simulations of Correlated Primary Radiation Defects in Ionic Solids. - Abstr. Latv. Phys. Soc.Conf., 1994, Daugavpils, p.19.

A-63. Heifets E., Orlando R., Dovesi R., Pisani C., and Kotomin E.A. *ab initio* Simulation of the Ag/MgO Interface. - Abstr.2nd Int.Conf. on Computer Simulations of Radiation Effects in Solids, 1994, Santa Barbara, p.87.

A-64. Kotomin E.A., Jacobs P.W.M., and Stashans A. Atomistic Modelling of Point Defects in Corundum Crystals. - Ibid., p.93-94

A-65. E.A.Kotomin and A.I.Popov. Computer Simulations of Correlated Annealing of Primary Radiation Defects in Alkali Halide Crystals. - Ibid., p.95.

A-66. Kotomin E.A. and Popov A.I. Computer Simulations of Correlated Annealing of Primary Radiation Defects in Alkali Halide Crystals. - Abstr.Eur. Res. Conf.on Electronic Structure of Solids, 1994, Gausdal, Norway, p.54.

A-67. Kotomin E.A. Semi-empirical Simulations of Defects in Oxide Crystals.- Abstr. IX Nordic Symp. on Computer Simulations of Solids, Göteborg, 1995. P.14.

A-68. Kotomin E.A. and Kuzovkov V.N. Aggregation Kinetics of Interacting Particles with a Permanent Source. - Abstr.Symp. on Dynamical Processes in Condensed Molecular Systems, Baden/Vienna, 1995, P.38.

A-69. Kuklja M.M., Kotomin E.A., and Popov A.I. Diffusion of Electron Centers in Ionic Crystals: Semi-Empirical Simulations. - Abstr.$G-IV/P27$ of Symp.G, Euro-MRS Meeting, Strasbourg, 1995.

A-70. Kotomin E.A. and Kuzovkov V.N. Microscopic Theory of Colloid Formation in Solids Under Irradiation. - Ibid., Abstract $G-III-3$.

A-71. Heifets E., Kotomin E.A., Dovesi R., and Pisani C. Hartree-Fock Simulations of the Ag/MgO Interface Structure. -Ibid., Abstract $G-I.6$.

A-72. Kotomin E.A., Kuklja M.M., Eglitis R.I., Stashans A., and Popov A.I. The Electronic and Atomic Structure of Single and Dimer Electron Defects in MgO and Corundum Crystals. - Abstr. Conf.on Rad. Effects in Insulators (REI-8), Catania (Italy), 1995, P.196.

A-73. Svane A., Kotomin E.A., and Schultz W. First-Principles Calculations of the Vibrational Properties of H Centers in KCl Crystals. - Ibid, p.203.

A-74. Jacobs P.W.M. and Kotomin E.A. Calculations of the Migration and Aggregation Energies for Radiation Defects in MgO Crystals.- Ibid., p.193.

A-75. Kuklja M.M., Kotomin E.A., and Popov A.I. Semi-Empirical Simulations of the Diffusion of Electron Centers in MgO Crystals. - Ibid., p.197.

A-76. Kuzovkov V.N. and Kotomin E.A. Microscopic Theory of Colloid Formation Under Irradiation. - Ibid., p.198.

A-77. Kotomin E.A. Semi-Empirical Simulations of Defects in MgO and Corundum Crystals. - Abstr.Danish Phys. Soc. Meeting, Odense, 1995, p.20.

A-78. Kotomin E.A. Microscopic Theory of Radiation-Induced Colloid Formation. -Ibid., p.30.

A-79. Heifets E., Dovesi R., Pisani C., and Kotomin E.A. The atomic and electronic structure of the Ag/MgO interface. - Abstr. 1995 Fall MRS Meeting, Symposium P (Materials Theory), Boston, p.478.

A-80. Kotomin E.A., Svane A., Brudevoll T., Schulz W., and N.E.Christensen, First-principles simulations of interstitial atoms in ionic solids. - Ibid, p.474.

A-81. Kotomin E.A., Svane A., Brudevoll T., and Christensen N.E. Electronic structure and diffusion mechanism of interstitial atoms in KCl and MgO crystals. - Abstr. Amer. Phys. Soc. Meeting (March 1996, San Louis), p. 129, C21-9.

A-82. Grigorjeva L., Millers D., and Kotomin E.A. The kinetics of excitonic luminescence in silver halides. - Abstr. Sov. Conf.on Scintillating Materials (SCIMAT-96, Ekaterinburg, 1996), p. 19

A-83. Puchin V.E., Shluger A.L., Kotomin E.A., Günster J., Brause M. and Kempter V. Atomic structure of the (0001) corundum surface. - Abstr. Int. Conf. on Defects in Insulating Materials (ICDIM-96, Winston-Salem, USA, July 96), p. 44.

A-84. Kotomin E.A. and Kuzovkov V.N. The kinetics of radiation-induced defect accumulation in ionic solids. - Ibid. p. 100.

A-85. Jacobs P.W.M., Kotomin E.A., Christensen N.E., Brudevoll T. and Kuklja M.M. Theory of diffusion and aggregation of radiation-induced defects in MgO and corundum crystals. - Ibid., p. 101.

A-86. Eglitis R.I., Kotomin E.A., Devreese J.T. and Popov A.I. The atomic and electronic structure of bound hole polarons and bipolarons in MgO crystals. - Ibid., p. 237.

A-87. Popov A.I. and Kotomin E.A. A mechanism of the$F^+ \to F$ center photoconversion in oxides. - Ibid., p. 247.

A-88. Popov A.I. and Kotomin E.A. A simple relation for the H_A center destruction temperatures in doped alkali halide crystals. - Ibid., p. 205.

A-89. Stashans A., Popov A.I. and Kotomin E.A. Semi-empirical simulations of close cation Frenkel pairs in corundum crystals. - Ibid., p. 245.

A-90. Heifets E. and Kotomin E.A. The adhesion energy of Ag/MgO interface: Hartree-Fock study. - Ibid., p. 210.

A-91. Kuzovkov V.N. and Kotomin E.A. Theory of diffusion-controlled colloid formation in irradiated solids. - Abstr.3- PO-187 at the 13 Int. Conf. on Reactivity of Solids, Hamburg, September 1996.

A-92. Jacobs P.W.M., Kotomin E.A., Kuklja M.M., Eglitis R.I., Stashans A. and Popov A.I. Semi-empirical calculations of luminescence properties of point defects in MgO and corundum crystals. - Int. Conf. on Luminescence (ICL, Prague, August 96), Abstr. P8-162.

A-93. Grigorjeva L., Millers D.K., Popov A.I., Kotomin E.A. and Polzik E.S. Luminescence Properties of $KNbO_3$ crystals. - Ibid., Abstr.P8-155.

A-94. Grigorjeva L., Millers D.K. and Kotomin E.A. Excitonic luminescence in silver halide crystals and fibers. Ibid., Abstr. P-13-88.

A-95. Kotomin E.A., Jacobs P.W.M., Christensen N.E., Brudevoll T., Kuklja M.M and Popov A.I.. Calculations of the diffusion and aggregation energies for intrinsic defects in MgO and corundum. - Abstr. Int. Conf. on Diffusion in Materials (DIMAT, Nordkirchen, August 96), p. 280.

A-96. Kuzovkov V.N. and Kotomin E.A. Microscopic theory of diffusion-controlled defect aggregation under irradiation of solids. - Ibid., p. 314.

A-97. Heifets E. and Kotomin E.A. The adhesion nature of Ag/MgO interface. - Abstr. W 7.5 at the Spring MRS Meeting (San Francisco April 96), Symposium **W** (Computational Materials Science), p. 107.

A-98. Kotomin E.A., Eglitis R.I., Kuklja M.M. and Kantorovich L.N. , Ibid., W 8.8., p. 107.

A-99. Kotomin E.A. Large-scale computer simulations of optical properties of defects in oxide solids. - Abstr. Int. Conf. on Advanced Optical Materials (AOMD-96, Riga, August 96), p. 151.

A-100. Grigorjeva L., Millers D. and Kotomin E.A. Mechanisms of defect creation and recombination in silver halides. - Ibid., p. 84.

A-101. Heifets E., Kotomin E.A., Dorfman S., Fuks D. and Gordon A. [001] surface polarization of smart optical materials: atomistic study. - Ibid., p. 80.

A-102. Eglitis R.I. and Kotomin E.A. Calculations of F centers in $KNbO_3$ ferroelectric crystals. - Ibid., p. 156.

A-103. Zhukovskii Yu.F., Kotomin E.A., Nieminen R., Devreese J.T., and Stashans A. Quantum chemical simulations of bound hole polarons (V_{Mg} centers) in corundum crystals. - Ibid., p. 157.

A-104. Jacobs P.W.M., Kotomin E.A. and Evarestov R.A. Formation, diffusion and aggregation of radiation-induced defects in MgO and $\alpha - Al_2O_3$ crystals. - Ibid., p. 152.

A-105. Heifets E., Dorfman S., Fuks D., and Kotomin E. Atomic simulation of the (001) surface in $BaTiO_3$. - Abstr. of EuroMRS-96, Symposium B (Thin film materials), p. 340.

A-106. Kotomin E.A. and Kuzovkov V.N. The kinetics of diffusion-controlled $A + B \rightarrow 0$ reaction in condensed matter: efects of non-equilibrium charge screening. - Abstr. NORDITA workshop on statistical physics Copenhagen, May 1996, P-20

A-107. Zhukovskii Yu.F., Kotomin E.A. and Nieminen R.M. - Quantum chemical simulations of defects in corundum crystals. - Abstr. X-th Nordic Symposium on Computer Simulations, Tallin, June 1996, p. 25.

A-108. Heifets E. and Kotomin E.A. The adhesion nature of Ag/MgO interface: Hartree-Fock study. - Ibid., p. 52.

A-109. Kotomin E.A. and Kuzovkov V.N. Theory of diffusion-controlled point defect aggregation during irradiation. - Abst. of Symposium B of the Fall MRS Meeting, Boston 1996, p. 63.

A-110. Kuzovkov V.N. and Kotomin E.A. Pattern formation and unusual reaction kinetics between charged reactants in low dimensions. - Ibid., Symp. EE, p. 667.

A-111. Puchin V., Kotomin E.A. and Shluger A.L. Atomic and electronic structure of the corundum (0001) surface. - Ibid., Symp.R, p. 460.

A-112. Heifets E., Kotomin E.A., Fuks D., Dorfman S. and Gordon A. Atomistic study of surface polarization of superconducting perovskites. - Ibid., Symp. Ca., p. 84.

A-113.Heifets E., Kotomin E.A., Fuks D., Dorfman S. and Gordon A. Surface structure of ferroelectric perovskites. -Ibid., Symp. Y, p. 569.

A-114. Heifets E. and Kotomin E.A. The adhesion nature of Ag/MgO interface: Hartree-Fock study. - Ibid., p. 537.

A-115. Kotomin E.A., Christensen N.E., and Eglitis R. A comparative study of the atomic and electronic structure of defects in oxide crystals: ab initio and semi-empirical study. Abstr. of Symp. D, European MRS, Strasbourg, June 1997, p.34

A-116. Kotomin E.A. and Kuzovkov V.N. The microscopic theory of diffusion-controlled defect aggregation. -Ibid., p.23

A-117. Zhukovskii Yu.F., Heifets E., Kotomin E.A., and Nieminen R.M. Ab initio study of the electronic and atomic structure of the Ag/MgO interface. - Ibid., p.45

A-118. Zhukovskii Yu.F., Alfredsson M., Heifets E., Hermansson K., Kotomin E.A., and Nieminen R.M. Ab initio Hartree–Fock simulations of silver film adhesion on both corundum and MgO (001) surfaces. - Abstr. 11 Nordic Symp on Computer Simulations, Copenhagen, June 1997. P.26.

A-119. Zhukovskii Yu.F., Heifets E., Kotomin E.A., and Nieminen R.M. Ab initio study of the electronic and atomic structure of the Ag/MgO interface.-. Abstr. 7 Europ.Conf. on Applications of Surfaces and Interface Analysis. Goteborg, June, 1997, Abstract AD-14, p.418.

A-120. Zhukovskii Yu.F., Alfredsson M., Hermansson K., Kotomin E.A., and Nieminen R.M. Ab simulations of CO adsorption on both clean and Ag-predosed (0001) corundum surfaces. - Ibid., Abstr. CA-15, p. 335.

A-121. Kotomin E.A. and Eglitis R.I. Charge distribution and optical properties of F and F^+ centers in $KNbO_3$ ferroelectric crystals. - Abstr. Int. Conf. on Defects in Semiconductors, Portugal, July 1997, p.38

A-122. Eglitis R., Kotomin E.A., Popov A.I. Atomic calculations of F-centers in ferroelectric $KNbO_3$ crystals. - Abstr.4th Intern.MRS Conf.in Asia, Chiba, Japan, Sept. 1997, Symposium R, p.20

A-123. Heifets E., Zhukvskii Yu., and Kotomin E.A., Ab initio Hartree-Fock Simulations of Silver Film Adhesion on both A_2O_3 (0001) and MgO (001) surfaces. – Int. Conf. Comput. Phys., California, 1997, session L, p. 30

A-124. Kotomin E.A. and Popov A.I. Radiation-Induced Point Defects in Simple Oxides. - Abst. Int. Conference on Radiation Effects in Insulators (REI-9), 1997, p.1

A-125. Zhukovskii Yu.F., Kotomin E.A. and R.M. Nieminen. Quantum Chemical Simulations of Bound Hole Polarons in Corundum Crystals. - Ibid., p.3a

A-126. Huisinga M., Bouchaala N., Bennewitz R., Reihling M., Kotomin E.A., Matthias E., Kuzovkov V.N., and von Niessen W. The kinetics of CaF_2 Metalization Induced by Low-Energy Electron Irradiation. - Ibid., p.4

A-127. Zhukovskii Yu.F., Heifets E., and Kotomin E.A. *Ab initio* simulations of silver film adhesion on A_2O_3 (0001) and MgO (001) surfaces. - Ibid., p.3b

A-128. Kotomin E.A., Kuklja M.M., Popov A.I., Christensen N.E., and Jacobs P.W.M. Theory for Radiation Defect Diffusion in Ceramic Materials. - Abstr. 10th Int. Conf. on Surface Modification of Metals by Ion Beams. - Gatlinburg, Tennesee, 1997. p.15

A-129. Kotomin E.A. and Popov A.I. Kinetics of correlated recombination of radiation defects in ionic solids. - Abstr. European Research Conf. on Particle-Solid Interactions: Strong Perturbations. San Sebastian, 1997. p. 20

A-130. Kotomin E.A. and Eglitis R.I. Quantum Chemical Simulations of Perovskite Surface Relaxation and Optical Properties for F centers therein. - Abstr. 13 conf. of the Inst. of Solid State Physics, Univ. of Latvia, Riga, 1997, p.49.

A-131. Eglitis R.I., Kotomin E.A., Postnikov A.V., Christensen N.E., and Borstel G. First-principles and semi-empirical calculations for the F centers in $KNbO_3$ and Li impurity in $KTaO_3$. Abstr. 5th Williamsburg Int. Workshop On First-Principles Theory of Ferroelecticity, 1998, p. 22.

A-132. Eglitis R.I., Kotomin E.A., Postnikov A.V., Christensen N.E., Borstel G., Philpott M.R. Computer simulations of defects in perovskite $KNbO_3$ crystals. - Abstr. 2nd Asian Meeting on Ferroelectrics, Singapore, 1998, p.45

A-133. Kuzovkov V.N., Kotomin E.A., von Niessen W. Theory of diffusion-controlled Frenkel defect aggregation. - Abstr.No To249:Poo7/23 at the 20th IUPAP Int. Conf. on Statistical Physics, Paris, 1998.

A-134. Millers D.K., Grigorjeva L., Kotomin E.A. Primary Radiation Defect Creation and Separation in AgBr. - Abstr. Int. Conf. Defects in Insulating Materials, Keele, 1998, p.20

A-135. Jacobs P.W.M., Kotomin E.A., Eglitis R.I. Semi-empirical INDO and shell-model calculations for perovskites. - Ibid., p.98

A-136. Yohum H.M., Ucer K.B., Williams R.T., Sheldon P.A., Nagirnyi A., Denks V., Grigorjeva L., Millers D.K., Kotomin E.A. Short- pulse excitation and spectroscopy of $KNbO_3$, $LiNbO_3$ and $KTiPO_4$ Ibid.129.

A-137. Kotomin E.A. and Zhukovskii Yu. Ab initio calculations of the metal/oxide interfaces. - Abst. 10th Nordic Symposium on Computer Simulations, 1998, Finland, p.20.

A-138. Kotomin E.A., Eglitis R.I., Borstel G. Quantum chemical modelling of point defects in $KNbO_3$ perovskite crystals. - Euro-MRS Meeting, Symposium C, Strasburg 1999, p. C-3.

A-139. Kalnin J.R. and Kotomin E.A. The effective diffusion coefficient in inhomogeneous solids. - Abstr. Int. Conf. on Radiation Effects in Insulators-10, Jena 1999, p.111

A-140. Kotomin E.A., Eglitis R.I., Borstel G., Grigorjeva L.G., Millers D.K., Pankratov V. - Theoretical and Experimental Study of Radiation Defects in $KNbO_3$ Perovskite Crystals. - Ibid., p.154.

A-141. Heifets E., Kotomin E.A., and Borstel G. Atomistic Simulations of the (110) Surface Relaxation for Perovskite Titanates. - Abstr. ICSOS-6 (Int. Conf. on Surfaces, Vancouver July 1999), p.33.

A-142. Zhukovskii Yu., Kotomin E.A., Dorfman S., Fuks D. Microscopic Modelling of Metal-Oxide Interfaces. - Abst. Int. Conf. on Interfacial Phenomena in Composite Materials, Berlin, Sept.99, p. 33.

A-143. Borstel G., Kotomin E.A., Eglitis R.I., Heifets E. Computer Modelling of Defects and Surfaces in Advanced Perovskites. Abstr. Int. Conf. Ternary and Multinary Compounds (ICTMC-12), 2000, Taiwan, p.23.

A-144. Eglitis R.I., Kotomin E.A., Borstel G. Quantum Chemical Modelling of Point Defects and Perovskite Solid Solutions. – Abstr. 2nd Int.Meeting on Predictive Process Simulations (ChiPPS), Wandlitz-Berlin, June 2000, p.29.

A-145. Kotomin E.A., Kuzovkov V.N., Popov A.N. The Kinetics of Defect Aggregation and Metal Colloid Formation in Insulating Solids under Irradiation. - Abstr. ICDIM Johannesburg April 2000, p.77.

A-146. Kashcheyevs V., Kotomin E.A., Kuzovkov V.N. Modelling of Metal Colloid Formation in Tracks of Swift Heavy Ions in Ionic Solids. - Ibid., p.50.

A-147. Kuzovkov N.V., Popov A.I., Kotomin E.A., Monge M.A., Gonzalez R., Chen Y. The Kinetics of F-Center Aggregation in Thermochemically Reduced MgO Single Crystals. - Ibid., p.183.

A-148. Borstel G., Kotomin E.A., Eglitis R.I., Heifets E. Computer Modelling of Point Defects, Impurity Self-Ordering Effects and Surfaces in Perovskite Ferroelectrics. - Abstr. Int. Conf. on Condensed Matter Physics, (Jaszowiec 2000, Poland), p. 20.

A-149. Kalnin J.R., Kotomin E.A., Kuzovkov V.N. The Effective Diffusion Coefficient in Inhomogeneous Solids. - Abstr. Vth Int. Conf. on Diffusion in Materials, Paris, July 2000, p. 182.

A-150. Heifets E., Kotomin E.A. Calculation of surface relaxation for perovskite crystals. - Abstr. MRS Fall meeting, Boston, December 2000, Symposium, p. 23.

A-151. Zhukovskii Yu., Kotomin E.A., Fuks D., Dorfman S., Gordon A. Hartree–Fock study of adhesion and charge distribution on the Ag/MgO (001) interface. Abstr. Int. Conf. ICSOS-9, Madrid, July 2000, p. 345.

A-152. Borstel G., Eglitis R.I., Kotomin E.A., Computer modeling of KTN solid solutions. - Abstr.12th IEEE International Symposium on the Application of Ferroelectrics, ISAF 2000, Hilton Hawaiian Village, Honolulu, Hawaii, USA, July 30 - August 2, 2000, p.20.

A-153. Eglitis R.I., Kotomin E.A., and Borstel G., Computer modelling of ABO_3 perovskites, Psik-2000 Conference on em Ab initio (from electronic structure) calculations of complex processes in Materials, Schwbisch Gmnd, August 22-26,2000, p. 126.

A-154. Vikhnin V.S., Eglitis R.E., Kotomin E.A., Kapphan S.E., Borstel G. New polaronic-type excitons in ferroelectric oxides. Abstr. Workshop on Fundamental Physics of Ferroelectrics, Williamsburg, USA, February 4-7, 2001. p.23

A-155. Heifets E., Cohen R.E., Eglitis R.I., Kotomin E.A., Borstel G. First- principles and semi-empirical calculations of atomic and electronic structure for $SrTiO_3$ (100) and (110) surfaces. - Abstr. APS meeting (Seattle, March 12-16, 2001), p.23.

A-156. Eglitis R.I., Kotomin E.A., and Borstel G. Computer modeling of luminescence in ABO_3 perovskites. Abstr. MRS Spring meeting (San Francisco, April 16-20, 2001), p. 142.

A-157. Vikhnin V.S., Eglitis R.I., Kotomin E.A., Kapphan S.E., Borstel G. New polaronic-type excitons in ferroelectric oxides. - ibid., 435.

A-158. Heifets E., Cohen R.E., Eglitis R.I., Kotomin E.A., Borstel G. Calculations of surface structure for $SrTiO_3$ perovskites. - ibid. p.289.

A-159. Kotomin E.A., Eglitis R.I., Maier J., Heifets E. Calculations of the atomic and electronic structure for ABO_3 thin films. - Abstr. E-MRS meeting, Strasburg, June 5-8, 2001, Symp. N., p.N-12.

A-160. Kotomin E.A., Evarestov R.A. Large-scale ab initio modelling of defects in perovskites: Fe impurity in $SrTiO_3$. Ibid., symp. A, p.A-1.

A-161. Dorfman S., Fuks D., Kotomin E.A., Zhukovskii Yu., Stoneham A.M. Theoretical analysis of the growth mode for thin metallic films on oxide surstrates. - Ibid., symp.A, p.A-I9.

A-162. Kotomin E.A. Atomistic theory of thin metal film growth on ionic surstrates. - Abstr. NATO Advanced Research Workshop on Atomic Aspects of the Epitaxial Growth, Corfu, July 26-31, p.16.

A-163. Kotomin E.A., Eglitis R.I., Borstel G. Calculations of radiation- induced point defects, polarons and excitons in ferroelectric perovskites. - Abstr. 11 Intern. Conf. on Radiation Effects in Insulators, Lisbon, September 3-9, 2001, p. 44.

A-164 Gonzalez R., Kotomin E.A., Popov A.I., Kuzovkov V.N. Diffusion-controlled annihilation and aggregation of F-centers in thermochemically reduced MgO crystals.- Ibid., p. 116.

A-165. Hermansson K., Herschend B., Zhukovskii Yu., Kotomin E.A., and Jacobs P.W.M. Metal-oxide bonding in the Ag/MgO (100) interface: an effect of metal coverage. - Abstr. Europ. Conf. on Molec. Mechanisms of Heterog. Catal., San Feliu de Guixols (Spain), 2001, p. 24.

A-166. Zhukovskii Yu., Kotomin E.A., Herschend B., Hermansson K., and Jacobs P.W.M. The adhesion properties of the Ag/a-Al_2O_3 (0001) interface: an ab initio study. – Ibid., p. 58.

A-167. Eglitis R.I., Kotomin E.A., and Borstel G. Computer modelling of point defects in perovskite crystals. – Abstr. 10 Intern. Meeting on Ferroelectricity (Madrid, September 3-7, 2001), p.44

A-168. Vikhnin V.S., Eglitis R.I., Kapphan S.E., Kotomin E.A., and Borstel G. New Type Charge Transfer Excitons in Ferroelectric Oxides. – Ibid., p. 61.

A-169. Eglitis R.I., Kotomin E.A., Borstel G., Heifets E., and Cohen R.E. Ab initio calculations of atomic and electronic structure for $SrTiO_3$ (100) surfaces. – Ibid., p. 69.

A-170. Eglitis R.I., Vikhnin V.S., Kapphan S.E., Kotomin E.A., and Borstel G. Structure and recombinational luminescence of polaronic-type excitons in ferroelectric oxides. – Ibid., p. 80.

A-171. Kotomin E.A., Maier J., Zhukovskii Yu.F., Fuks D., and Dorfman S. Ab initio Modelling of Silver Adhesion on the Corundum (0001) Surface. – Abstracts EMRS, Symp. Q, Strasburg, June 18-21, 2002, p. Q-7.

A-172. Fuks D., Dorfman S., Kotomin E.A., Zhukovskii Yu.F., and Stoneham A.M. Theoretical Conditions for the Initial Stages of the Effective Growth of High Quality Metal Films. – Ibid., Symp. J, p. J-3.

A-173. Eglitis R.I., Heifets E., Kotomin E.A., Maier J., and Borstel G. First-principles Calculations for Perovskite Thin Films. – Ibid., Symp. P, p. P-3.

A-174. Eglitis R., Fuks D., Dorfman S., Kotomin E.A., and Borstel G. Large-scale Modelling of the Phase Transitions in KTN Perovskite Solid Solutions. – Ibid., Symp. P, p. P-3.

A-175. Eglitis R., Kotomin E.A., Kapphan S.E., Vikhnin V.S., and Christensen N.E. Calculations of the Electronic and Atomic Structure of Point Defects, Polarons and Excitons in ABO_3 Perovskite Crystals. – Ibid., symp. A, p. A-7.

A-176. Eglitis R., Heifets E., Kotomin E.A., and Borstel G. Calculations of Atomic and Electronic Structure for (100) Surfaces of $SrTiO_3$ Perovskite. – Abstracts MRS Spring-2002 Meeting, San Francisco, April 1-5, 2002, p. 113.

A-177. Eglitis R., Kotomin E.A., Christensen N.E., and Borstel G. Calculations of the Electronic and Atomic Structure and Diffusion of Point Defects in $KNbO_3$ Perovskite Crystals and Relevant KTN Solid Solutions. – Ibid, p.117.

A-178. Evarestov R.A., Eglitis R., Piskunov S., Kotomin E.A., and Borstel G. Large scale ab initio Simulations of Fe-doped $SrTiO_3$. – Ibid., p.395.

A-179. Eglitis R., Vikhnin V.S., Kotomin E.A., Kapphan S.E., and Borstel G. Theoretical Prediction and Experimental Confirmation of Charge Transfer Vibronic Excitons and Their Phase in ABO_3 Perovskite Crystals. – Ibid., p. 116.

A-180. Kotomin E.A., Maier J., Stoneham A.M., Zhukovskii Yu.F., Fuks D., and Dorfman S. Ab initio Modelling of Metal Adhesion to Ceramics. – Abstracts CIMTEC–10 (International Ceramics Congress, Florence, July 15-18, 2002, Techna Publishers), p. 58.

A-181. Fuks D., Dorfman S., Zhukovskii Yu.F., Kotomin E.A., and Stoneham A.M. Thermodynamics of the Initial Stage of Growth for a Thin Metallic Film on an Insulating Substrate. – Ibid., p. 58.

A-182. Zhukovskii Yu.F., Kotomin E.A., and Jacobs P.W.M. Large scale computer simulations of metal/oxide interfaces with defects. – Abstracts of AOMD-3 (Int. Conf. on Advanced Optical Materials and Devices, August 19-22, 2002, Jurmala, Latvia), p. 38.

A-183. Borstel G., Eglitis R., and Kotomin E.A. Computer modelling of point defects, polarons and excitons in perovskite ferroelectrics. – Ibid., p. 29.

A-184. Piskunov S., Evarestov R.A., Kotomin E.A., Eglitis R., and Borstel G. Large scale first-principles calculations of Fe-doped $SrTiO_3$. – Ibid., p. 31.

A-185. Heifets E., Eglitis R.I., Kotomin E.A. and Borstel G. *Ab initio* Calculations for $SrTiO_3$ (100) Surface Structure. – Abstracts of Williamsburg Meeting on Fundametal Physics of Ferroelectrics– 2002, p.20.

A-186. Eglitis R.I., Kotomin E.A., Borstel G., Vikhnin V.S. Quantum chemical Modelling of Polarons and Excitons in ABO_3 Perovskites. – Abstr. Int. Workshop on Fundamental Physics of Ferroelectrics, Williamsburg 2003, p.32.

A-187. Eglitis R.I., Fuks D., Dorfman S., Kotomin E.A., Borstel G., Trepakov V.A. Quantum chemical modelling of phase transitions in perovskite solid solutions. – Ibid., p.33.

A-188. Heifets E., Eglitis R.I., Kotomin E.A., Maier J., and Borstel G. Ab initio calculations of the polar surface structure for $SrTiO_3$ perovskite. — Ibid., p.43.

A-189. Heifets E., Evarestov R.A., Kotomin E.A., Dorfman S. Modelling of Polar (110) Oxygen-terminated Surface of $LaMnO_3$ — Abstr. E-MRS Meeting, Strasburg, June 2003, Symp.N: New Materials and technologies in sensor applications, p. N20.

A-190. Zhukovkii Yu., Kotomin E.A., Fuks D., Dorfman S., Stoneham A.M., Borstel G. First-principles simulations of 2D Cu superlattices on MgO. — Ibid., symp.F: Nanostructures from clusters, p. F13.

A-191. Eglitis R.I., Heifets E., Kotomin E.A., Maier J., and Borstel G. Ab initio modelling of the atomic and electronic structure of $SrTiO_3$ polar surface. — Abstr. EMF-2003 (10th Euro-meeting on Ferroelectricity, Cambridge, UK, August 3-8, 2003), p. 120

A-192. Eglitis R.I., Kotomin E.A., Borstel G., Fuks D., Dorfman S. and Trepakov V.A. Quantum chemical modelling of the atomic and electronic structure of ABO_3 perovskites. — Ibid., p.121.

A-193. E.A. Kotomin, J. Maier, and E. Heifets. Hartree– Fock Calculations of the Surface Structure for ABO_3 Perovskites. – Abstr. Int. workshop on Problems of Computational Physics, St.Petersburg, 25-28 August 2003, p.6.

A-194. E.A. Kotomin, J. Maier, E. Heifets, and R. Eglitis. First principles calculations of the surface structure for ABO_3 perovskites. – Abstr. 9th Int. Conf. on Solid State Chemistry, Stuttgart, 3-6. Sept. 2003, P046.

A-195. R. Merkle, J. Maier, E.A. Kotomin, J. Purans. Joint theoretical and experimental studies of polycrystalline $SrTiO_3$. – Ibid., P047.

A-196. O. Sychev, Yu. F. Zhukovskii, E.A. Kotomin, and G. Borstel. Ab initio calculations of copper nanostructures on oxide substrates. – Abst. Fall- EMRS Meeting, Symp. F, Warzawa, Sept. 2003, p.23.

A-197. E. Heifets, R.A. Evarestov, E.A. Kotomin, S. Dorfman and J. Felsteiner. Surface relaxation and rumpling of the (110) oxygen-terminated surface of $LaMnO_3$. – Abstr. 1st Int. Meeting on Applied Physics (APHYS-2003), Badajoz, Spain, 14-18 October 2003, p.10.

A-198. S. Piskunovs, G. Borstel, S. Dorfman, E.A. Kotomin, and D. Fuks. Quantum chemical calculations of $BaSrTiO_3$ solid solutions. – Ibid., p.12.

A-199. Kotomin E.A., Kalnin J.R., and Maier J. Abstr. 85th Bunsen Colloquium, 31.October 2003, Abstracts, p. 25.

A-200. R.I. Eglitis, S. Piskunov, E. Heifets, E.A.Kotomin, and G. Borstel. Ab initio study of $SrTiO_3$, $BaTiO_3$ and $PbTiO_3$ surfaces. – Abstr. 2nd Int. Conf. on Materials for Advanced Technologies, Singapore, December 2003, p.20.

A-201. R.I. Eglitis, E.A.Kotomin, and G. Borstel. Computer Modelling of Point Defects in ABO_3 Perovskites and MgO. – Ibid., p.35.

A-202. Kotomin E.A., E. Heifets, S. Dorfman, A. Gordon and D. Fuks. Atomistic Calculations of Perovskite Polar Surface Structures. – Abstr. Int. Conf. on Surface Science (ECOSS-22), Prague, September 2003, p.321.

A-203. Zhukovskii Yu., Kotomin E.A., Dorfman S., Fuks D. First principles simulations on the regular Cu/MgO(100) interface. – Ibid., p.200.

A-204. Dorfman S., Piskunov S., Kotomin E.A., Fuks D. Calculations of the atomic and electronic structure of $BaSrTiO_3$ (BST) solid solutions. – Abstr. EMRS Spring Meeting, Strasburg, May 2004, Symposium D, Abstract D-II.4.

A-205. Fuks D., Dorfman S., Bakaleinikov L., Gordon A., Kotomin E.A. The electronic structure of perovskite magnanates. – Ibid., symposium K, Abstract K/P17.

A-206. Zhukovskii Yu., Kotomin E.A., Fuks D., Dorfman S. A comparative study of Ag and Cu adhesion on MgO (001) surface. – Ibid., Symposium T, Abstract T-VIII.03

A-207. Zhukovskii Yu., Kotomin E.A., Fuks D., Dorfman S. Ab initio study of the growth mode for thin Cu films on oxide substrates. – Ibid., Symposium G, Abstract G-XI.01

A-208. Zhukovskii Yu., Kotomin E.A., Mastrikov Yu., Maier J. Ab initio simulations on AgCl(111) surface and AgCl(111)/a-Al2O3 (0001) interface. – Ibid., Abstract H-P.26

A-209. Kotomin E.A. and Heifets E. First principles calculations of the atomic and electronic structure of ABO_3 surfaces. – Abstr. ESPA-2004 Conf., Spain, Valladolid, 15-17 Sept. 2004, p.6.

A-210. Eglitis R., Kotomin E.A. and Borstel G. Large scale computer modelling of point defects in ABO_3 perovskites. – Abstracts ICDIM-2004, Riga, July 2004, p.4 (invited talk).

A-211. Illas F., Lopez N., Carrasco J., Kotomin E., Zhukovskii Yu., Piskunov S., Maier J., and Hermansson K. First principles simulations of F centers in $SrTiO_3$ perovskite. – Ibid., p. 51.

A-212. Zhukovskii Yu. and Kotomin E.A. Transition metal adsorption on defective MgO (001) surface: ab initio study. – Ibid., p. 70.

A-213. Heifets E., Kotomin E.A., Evarestov R.A., Maier J. The ab initio atomic and electronic structure calculations for ABO_3 perovskite polar surfaces. – Abstr.H3.12 of Fall MRS meeting, Boston, November 2004, p.129.

A-214. Kotomin E.A., Illas F., Lopez N., Carrasco J., Zhukovskii Yu., Mastrikov Yu., Maier J. First-principles calculations of F centers in $SrTiO_3$ perovskites. – Ibid., Abstr. H11.10, p. 138.

A-215. Evarestov R.A., Kotomin E.A., and Zhukovskii Yu.F., DFT study of a single F center in a cubic $SrTiO_3$ perovskite: periodic model of aperiodic system. – Abstracts of

9th V.A.Fock Meeting on Quantum and Computational Chemistry (Velikiy Novgorod, Russia, May, 2005), p. 26.

A-216. Balaya P., Dolle M., Li H., Hu Y., Jamnik J., Zhukovskii YU.F., Kotomin E.A., and Maier J. Nanocrystallinity effects in lithium battery electrodes with RuO_2 as a model material. – Abstracts of the Lithium Batteries Discussion (LiBD-2005) "Electrode Materials" (Arcachon, France, May, 2005) p.72-73.

A-217. Balaya P., Bhattacharyya A., Jamnik J., and Kotomin E.A. Nano-ionics in the context of Li Batteries. Abstracts of 3rd International Conference on Materials for Advanced Technologies ICMAT 2005(Singapore, July 2005),p.4.

A-218. Eglitis R.I., Borstel G., Heifets E., Piskunov S., and Kotomin E.A. *Ab initio* calculations of the $SrTiO_3$, $PbTiO_3$, $BaTiO_3$ (001) and $BaTiO_3$ (110) surfaces, Ibid., p. 142.

A-219. Balaya P., Zhukovskii Yu.F., Dolle M., Kotomin E.A., Li H., and Maier J. Experimental and theoretical evidence for novel interfacial mechanism for lithium storage in nanocomposites. – Abstracts of 15th International Conference on Solid State Ionics (Baden-Baden, Germany, July, 2005),p. 164.

A-220. Fuks D., Felsteiner J., Bakaleinikov L., Gordon A., Kotomin E.A., Maier J., and Fleig J. Thermodynamic stability and chemical bonding in $(La7/8Sr1/8)MnO_3$, Ibid., P-257.

A-221. Purans J., Merkle R., Kuzmin A., Kotomin E.A., Mathon O., Vracar M., and Maier J. XAFS study with subpicometer accuracy: local structure of Fe in $SrFe_xTi_{1-x}O_{3-y}$, Ibid., P-489.

A-222. Zhukovskii Yu.F., Kotomin E.A., and Ellis D. First principles simulation on the defect-free Cu/BaTiO3(001) cubic interfaces. Abstracts of the The 8th International Conference on the Structure of Surfaces (ICSOS) (Munich, Germany, July, 2005), p. 155.

A-223. Fuks D., Zhukovskii Yu.F., Kotomin E.A., and Ellis D. Coin metal adsorbtion on perfect and defective MgO(001) surfaces: the electronic structure calculations and film growth thermodynamics. – Ibid.,p. 227.

A-224. Zhukovskii Yu.F., Kotomin E.A., Krischok S., Hoefft O., and Kempter V. A comparative analysis of electron spectroscopy and *ab initio* studies on Cu adsorbtion on MgO. Abstracts — ibid., p. 228.

A-225. Zhukovskii Yu.F., Kotomin E.A., Krischok S., Hoefft O., and Kempter V. A comparative analysis of electron spectroscopy and *ab initio* studies on Cu adsorbtion on MgO. Abstracts 25 European Conference on Surface Science, ECOSS-23 (Berlin, Germany, September 2005), p. 191.

A-226. Zhukovskii Yu.F., Kotomin E.A., Mastrikov Yu.A., and Maier J. *Ab initio* study of ionic conductivity on AgCl/a-Al_2O_3 (0001) interface. – Abstracts of the Psi-k Conference 2005 (Schaebisch Gmuend, Germany, September, 2005), p. 472.

A-227. Zhukovskii Yu.F., Kotomin E.A., Balaya P., and Maier J. First principles modelling of interfacial Li storage. Ibid., p. 473.

A-228. Kalnin J.R., Kotomin E.A., Maier J., and Kuzovkov V.N. Calculation of the effective diffusion coefficient for heterogeneous media. – Abstracts of International Conference on Diffusion Fundamentals (Leipzig, Germany, September, 2005), p. 142-143.

A-229. Kuzovkov V.N., Kotomin E.A., and Zvejnieks G. Modelling of diffusion-controlled pattern formation in thin metallic film growth on crystalline substrates. – Ibid., p. 156-157.

A-230. Ronchi C., van Uffelen P., Schubert A., Bruynooghe C., Laar J.V., Kotomin E.A., et al. The new nuclear fuel R+D plan of the JRC-ITU on uranium-plutonium-americium nitrides and carbides. - Abstracts of GLOBAL 2005 International Conference "Nuclear Energy Systems for Future Generation and Global Sustainability (Tsukuba, Japan, October, 2005), paper 5B-II, 391.

A-231. Kotomin E.A. and Popov A.I. Point defect aggregation and metallic colloid formation in ionic solids. Abstracts of Int. Conference on Nanoscience and Nanotechnology (Frascati, Italy, November, 2005), p. 58.

A-232. Kotomin E.A., van Uffelen P., and Ronchi C. Atomistic modeling of radiation and impurity defects in UN nuclear fuels. – Abstracts of Int. Workshop on Materials Models and Simulations for Nuclear Fuels (Washington D.C., USA, November, 2005).

A-233. Piskunov S., Kotomin E.A., Zhukovskii Yu.F., and Ellis D.E. Adsorption of atomic and molecular oxygen on the $SrTiO_3(001)$ surfaces: Computer simulations by means of hybrid density functional calculations and *ab initio* thermodynamics. – Abstracts of 2005 MRS Fall Meeting (Boston, USA, November-December, 2005),p. LL8.5.

A-234. Kotomin E.A., Zhukovskii Yu.F., and Mastrikov Yu. First-principles modeling of surfaces and reactivity of oxide- and ABO_3 perovskite surfaces. – Abstracts of 2nd Latvian conference on Functional materials and nanotechnologies (Riga, Latvia, March, 2006), p. 33.

A-235. Zhukovskii Yu.F. and Kotomin E.A. Theoretical simulation on the enhanced Li storage in the interfaces between transition metals and ionic lithium compounds used in Li batteries. –ibid., p. 83.

A-236. van Uffelen P., Kotomin E.A., Ciriello A., Rondinella V.V., Staicu D., Wiss T., Konings R., and Somers J. The multi-time-scale approach to MX fuels at ITU. — Abstracts of 5th European Workshop on Materials Models and Simulations for Nuclear Fuels, MMSNF-5 (Nice, France, June, 2006).

A-237. Kotomin E.A., Ashley N., Grimes R., van Uffelen P. , Mastrikov Yu., Zhukovskii Yu.F., and Rondinella V.V. Atomic scale modeling of nitride nuclear fuels. — ibid.

A-238. Kotomin E.A., Kuzovkov V.N., and Zhukovskii Yu.F. Modelling of defects and defect-induced processes. – Abstracts of EFDA (EURATOM) Monitoring meeting on Modelling of Radiation Effects (Garching, Germany, June, 2006).

A-239. Zhukovskii Yu.F., Kotomin E.A., Mastrikov Yu., Piskunov S., Tsemekhman K.L., and Ellis D.E. Ab initio simulations of isolated F centers in cubic $SrTiO_3$ perovskite. Abstracts of 8th International Conference on Computer Simulation of Radiation Effects in Solids, COSIRES-06 (Richland, WA, USA, June 2006), p. 42.

A-240. Zhukovskii Yu.F., Fuks D., Kotomin E.A., and Ellis D.E. Differences of metal film growth modes on perfect and defective MgO surface. Ibid., p. 109.

A-241. Balaya P., Zhukovshii Yu.F., Bekaert E., Menetrier M., Dolle M., Li H., Kotomin E.A., and Maier J. Interfacial lithium storage in nanocomposites: experimental and theoretical evidences.— Abstracts of 13th International Meeting on Lithium Batteries, IMLB-06 (Biarritz, France, June 2006), Nr 291.

A-242. Zhukovskii Yu.F., Piskunov S., Kotomin E.A. , Heifets E., and Ellis D.E. A comparative study of cubic $PbZrO_3$ and $SrTiO_3$ perovskites containing single F- centers: ab initio simulations. — Abstracts of 134th Faraday Discussion: Atomic Transport and Defect Phenomena in Solids (Guildford, UK, July, 2006), P13.

A-243. Fuks D., Zhukovskii Yu.F., Kotomin E.A., and Ellis D.E. Role of surface F-centers in formation of ultra-thin Ag and Cu films on the MgO(001) substrate. Ibid., P14.

A-244. Kotomin E.A., Mastrikov Yu., Zhukovskii Yu.F., van Uffelen P., and Rondinella V.V. First-principles modelling of defects in advanced nuclear fuels. – Abstracts of 10th Europhysical Conference on Defects in Insulating Materials, EURODIM-06 (Milano, Italy, July, 2006), OTuB1, p.10.

A-245. Fuks D., Kotomin E.A., Zhukovskii Yu.F., and Ellis D.E. Coin metal adsorption on perfect and defective MgO (001) surfaces. Ibid., p.27.

A-246. Kotomin E. Atomistic modelling of defects in UN using VASP. – Abstr. of International Workshop on First Principles Calculations of Nuclear Fuels (Karlsruhe, Germany, March, 2007).

A-247. Zhukovskii Yu.F.. Bocharov D., and Kotomin E.A. Oxygen chemosorption on the UN(001) surface: periodic DFT simulation.– Abstracts of the 5th International Conference "Information Technologies and Management, ITMT 2007 (Riga, Latvia, April, 2007), p. 9-10.

A-248. D. Fuks, Yu.F. Zhukovskii, and E.A. Kotomin. A role of surface defects in thin metallic film growth mode on oxide surfaces.– Abstract C49 at the International Conference on Radiation Effects in Insulators (REI-14) (Caen, France, August-September, 2007).

A-249. E.A. Kotomin, R.W. Grimes, D. Parfitt, D. Gryaznov, Yu.F. Zhukovskii, Yu. Mastrikov, P. van Uffelen, V.V. Rondinella, and R.J.M. Konings. First principles modelling of radiation defects in advanced nuclear fuels.— Abstract O3 at the same conference.

A-250. Yu.F. Zhukovskii, E.A. Kotomin, P. Balaya, and J. Maier. Enhanced interfacial lithium storage in nanocomposites of transition metals with LiF or Li_2O: experimental studies and theoretical simulations. — Abstracts of the 11th European Conference on Solid State Chemistry, ECSSC-XI (Caen, France, September, 2007), p. 58.

A-251. E.A. Kotomin, Yu.F. Zhukovskii, and J.Maier. Enhanced interfacial Li storage in nanocomposites - ab initio modeling.– Abstract at the Workshop of FP6 ALISTORE network on Nano-materials for negative electrodes in lithium batteries (Paris, France, October, 2007).

A-252. E.A. Kotomin, Yu.A. Mastrikov, and Yu.F Zhukovskii. First-principles modeling of nuclear fuels. – Abstract at Nuclear Cross-Over (NXO) workshop on nuclear fuels (Tokyo, Japan, February, 2008).

A-253. E.A. Kotomin, Yu.A. Mastrikov, Yu.F. Zhukovskii, S. Piskunov, and J. Maier. First-principles modelling of perovskite surface reactivity. Abstract at International Baltic Sea Region conference on Functional materials and nanotechnologies 2008 (Riga, Latvia, April, 2008).p. 19.

A-254. D. Bocharov, Yu. Zhukovskii, R.A. Evarestov, E.A. Kotomin, and A. Bandura. Atomic and molecular oxygen adsorption on the UN (001) surface. ibid., p. 87.

A-255. V. Alexandrov, R.A. Evarestov, E.A. Kotomin, A. Kuzmin, J. Purans, M. Vracar, R. Merkle, J. Maier, Theoretical and structural studies of charge ordering in CaFeO3 and SrFeO3. Ibid., Abstracts: p. 88.

A-256. S. Piskunov, E. Spohr, T. Jacob, E. Heifets, E.A. Kotomin, and D.E. Ellis. Thermodynamic stability of La1-xSrxMnO3 surfaces: calculations by means of hybrid density functional theory. Ibid., Abstracts: p. 181.

A-257. E.A. Kotomin, J. Maier, Yu.A. Mastrikov, and Yu.F. Zhukovskii. First-principles calculations of the solid oxide fuel cells and interfacial storage in Li batteries. 5. Baltic conference on Electrochemistry (Tartu, Estonia, April-May, 2008).Abstract I-7.

A-258. E.A. Kotomin, Yu.A. Mastrikov, E. Heifets, R. Merkle, J. Fleig, J. Maier, A. Gordon, and J.Felsteiner. First-principles modeling of SOFC cathode – Abstracts of 213th Meeting of American Electrochemical Socienty (Phoenix, AZ, USA, May, 2008).

A-259. E.A. Kotomin, Yu.F. Zhukovskii, P. Balaya, and J. Maier. Enhanced interfacial lithium storage in nanocomposites of transition metals with LiF or Li2O: experimental studies and theoretical simulations. Ibid. p.22.

A-260. Yu.F. Zhukovkii, E.A. Kotomin, S. Piskunov, and Yu.A. Mastrikov. The effect of oxygen vacancies on the atomic and electronic structure of cubic ABO3 perovskite bulk and the (001) surface: Ab initio calculations. – Abstracts of 9th International Symposium on Ferroelectricity, RCBJSF-9 (Vilnius, Lithuania, June, 2008).p. 33.

A-261. E.A. Kotomin, Yu.F. Zhukovskii, S. Piskunov, and D.Ellis. Hybrid DFT calculations of the F centers in cubic ABO3 perovskites. Abstracts of International workshop in Ab initio modelling of crystalline materials (Torino, Italy, September, 2008).p.11.

A-262. V. Alexandrov, E.A. Kotomin, R.A. Evarestov, and J. Maier. Ab initio study of bulk and surface iron defects in SrTiO3. Ibid.p.12.

A-263. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, and A. Moslang, "Simulation of yttrium oxide particle formation in iron in support of ODS steel development". 5th International Symposium on Fusion Technology, (Rostock, Germany, September, 2008). Abstracts: p. 226.

A-264. D. Gryaznov, E. Heifets, and E.A. Kotomin. VASP calculations for perfect and defective actinide nitrides and oxides. 7th International Workshop on Materials Models and Simulations for Nuclear Fuels (Karlsruhe, Germany, September, 2008).

A-265. D. Bocharov, Yu.F. Zhukovskii, and E.A. Kotomin. Interaction of the oxygen molecule with the UN(001) surface: Ab initio modeling.Ibid.

A-266. S.N. Rashkeev, E.A. Kotomin, Y.A. Mastrikov, and P. van Uffelen. First principles modelling of defect migration in uranium nitride and transuranus prediction of fuel performance. Ibid.

A-267. P. van Uffelen, and E.A. Kotomin. Using first principle calculations for nitride fuels in a fuel performance code.Ibid.

A-268. E.A. Kotomin, Yu.F.Zhukovskii, and J.Maier. First principles modelling of interfacial mechanism for Li storage in nanocomposites. Abstracts of XXVIII. International Workshop on Fundamentals of Li Based Batteries (Schloss Ringberg, Bayern, Germany, November, 2008).

A-269. Kotomin E.A., Zhukovskii Yu.F., and Piskunov S. Hybrid functional calculations of point defects in ABO3 perovskites. – 5th International conference on Quantum Theory of SOlids. Aarhus, Denmark, May 2009.

A-270. Kotomin E.A., Merkle R., Mastrikov Yu., Heifets E., and Maier J. First principles modelling of oxygen incorporation into SOFC cathode. - Bunsentagung (108.Annual Meeting of German Physical Chemistry Society), Koeln, 21-23. May 2009, p.75.

A-271. Kotomin E.A., Merkle R., Mastrikov Yu., Heifets E., and Maier J. First principles modeling of pathways for oxygen incorporation into SOFC cathode. - Abstr. 17th conference on Solid State Ionics, Toronto, July 2009, p.255.

A-272. Piskunov S., Heifets E., Jacob T., Kotomin E.A., and Spohr S. Hybrid density functional calculations of thermodynamic stability and oxygen adsorption on LaMnO3 and La1-xSrxMnO3 (001) surfaces. – Abstr. Int. Congress on Quantum Chemistry, Helsinki, Finland, August 2009.

A-273. Merkle R., Mastrikov Yu., Heifets E., Kotomin E.A., Kuklja M.,and Maier J. Oxygen incorporation reaction into mixed conducting perovskites: a mechanistic analysis for (La,Sr)MnO3 based on DFT calculations. – Abstr. 216th Electrochemical Society Meeting. Vienna, 4-9. October 2009.

A-274. Popov A., Kotomin E.A., Maier J. Basic properties of radiation-induced point defects in halides and oxides. – Abstr. 15th Int. conference on Radiation Effects in Insulators. Padova, Italy, 30.08-4.09.2009, p.47.

A-275. Kotomin E.A., Zhukovskii Yu., Piskunov S., Maier J. First principles calculations of point defects in ABO3 perovskites. – Ibid., p.49.

A-276. Li K.D., Wang L., Ewing R., and Kotomin E.A. Dynamics of microstructural evolution in electron irradiated fluor-apatite. – Ibid., p.109.

A-277. Kotomin E.A., Kuzovkov V.N., Zvejnieks G., Li K.D., Wang L. Void superlattice formation in electron irradiated CaF2: theoretical analysis. – Ibid., p. 118.

A-278. Rashkeev S., Kotomin E.A., Mastrikov Yu. First principles calculations of defect migration in UN nuclear fuels. – Ibid., p. 199.

A-279. Gryaznov D., Kotomin E.A., Rashkeev S., Maugeri E., and Wiss T. Radiation defects in oxide nucler fuels: first principles modeling and He release experiments. – Ibid., p.204.

A-280. Kotomin E.A., Zhukovskii Yu., Piskunov S., Mastrikov Yu., and Maier J. First-principles calculations of radiation defects in perovskites.– Abstr. 14th Int. conference on physics and chemistry of inorganic materials. Astana, Kazahstan, October 2009.

A-281. Kotomin E.A., Zhukovskii Yu., Fuks D., Ellis D., Maier J. First principles modeling of metal ceramic interfaces: growth mode and surface defects. – Abstr. Int. conf. Materials Science and technology-2009, Pittsburg, USA, October 2009, p. 58.

A-282. Kotomin E.A., Merkle R., Heifets E., Mastrikov Yu., Maier J. Modeling of Oxygen Incorporation Reaction into SOFC Cathode: A first principles study. – Ibid., p. 64.

A-283. Rashkeev S., Kotomin E.A., Mastrikov Yu. First Principles Calculations of Defect Migration in UN Nuclear Fuels. – Ibid., p. 112.

A-284. Kotomin E.A., Mastrikov Yu., Heifets E., Merkle R., Kuklja M., Maier J. First Principles Modeling of SOFC Cathode. – ibid., p. 135.

A-285. Kotomin E.A., Alexandrov V., Zhukovskii Yu., Piskunov S., Maier J. First principles calculations of the static and dynamic properties of oxygen vacancies in ABO3 perovskites. – Ibid. p. 123.

A-286. Yu.F. Zhukovskii, S. Piskunov, E.A. Kotomin and S. Bellucci, Growth mechanism for CNT bundle upon both flat and nanostructured Ni catalyst: ab initio simulations. Abstracts of II. International conference "Functional materials and nanotechnologies" FMNT 2010 (Riga, Latvia, March, 2010), 16 p.

A-287. E.A. Kotomin, Yu. Mastrikov, R. Merkle and J. Maier, Oxygen incorporation reaction into mixed conducting ABO3 - type perovskites for fuel cell applications. Ibid., p.22.

A-288. D. Bocharov, D. Gryaznov, Yu.F. Zhukovskii and E.A. Kotomin, First principles calculations on oxygen impurities incorporated in the vacancies of UN(001) substrate. Ibid., p. 37.

A-289. S. Piskunov, E.A. Kotomin, Yu.F. Zhukovskii and V. Alexandrov, First-principles modeling of oxygen interaction with ABO3 type perovskite surfaces. Ibid., p.38.

A-290. D. Gryaznov, R.A.Evarestov, E.A.Kotomin and J.Maier, Electronic, phonon and magnetic structure of pure and Sr-doped LaCoO3. Ibid., p.39.

A-291. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin and A. Moeslang, Ab initio calculations of yttrium and vacancy point defects for ODS steels modeling. Ibid., p. 182.

A-292. P. Merzlakovs, G. Zvejnieks, V.N. Kuzovkov, E.A. Kotomin, K.D. Li and L.M. Wang, Analysis of void superlattice formation in CaF2. Ibid., p.185.

A-293. R. I. Eglitis and E.A. Kotomin, Ab initio calculations of Nb-doped SrTiO3. Ibid. p. 186.

A-294. R.I. Eglitis, A.F. Vassilyeva, E.A. Kotomin and A.K. Dauletbekova, Ab initio calculations of MgF2 (001) and (011) surfaces.Ibid., p. 187.

A-295. E.A. Kotomin, Yu.A. Mastrikov, M.M. Kuklja, R. Merkle, and J. Maier, First principles calculations of oxygen vacancy formation and migration in mixed conducting ABO3-type perovskites for solid oxide fuel cell applications. 9th International Symposium on Systems with Fast Ionic Transport, ISSFIT-9 (Riga, Latvia, June, 2010). Abstracts, p. 18.

A-296. R.I. Eglitis and E.A. Kotomin, Ab initio calculations of Nb-doped SrTiO3. VII. Spring European Materials Research Society (EMRS) Meeting (Strasbourg, France, June, 2010). Ibid., Abstract EP1-9.

A-297. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, and A. Mslang, Pair and triple point defect complex modeling in fcc Fe lattice. Ibid., Abstract NPVI-13.

A-298. D. Bocharov, D. Gryaznov, Yu.F. Zhukovskii, and E.A. Kotomin, Ab initio modeling of oxygen impurities incorporated within UN (001) surface and subsurface vacancies. Ibid., Abstract NPVI-23

A-299. R.A. Evarestov, Yu.F. Zhukovskii, S. Piskunov, M.V. Losev, A.V. Bandura, and E. Spohr, Symmetry and models of single- and double-walled titania nanotubes: comparative analysis using ab initio calculations. Ibid., Abstract PP8-6.

A-300. S. Piskunov, Yu.F. Zhukovskii, and E.A. Kotomin, Atomic carbon adsorption on nano-structured Ni catalyst and further CNT growth: Predictions from first principles calculations. Ibid., Abstract PP8-50.

A-301. E.A. Kotomin, and D. Gryaznov, DFT+U calculations of the electronic structure of perfect and defective PuO2. VIII. CECAM Conference on Actinides: Correlated Electrons and Nuclear Materials (Manchester, UK, June 2010). Abstracts, p.7.

A-302. R.I. Eglitis and E.A. Kotomin, Ab initio calculations of Nb impurity in SrTiO3. – 11th Europhysical Conference on Defects in Insulating Materials, EURODIM-2010 (Pecz, Hungary, July, 2010). Abstracts: 4.2.

A-303. R.I. Eglitis, A.F. Vassilyeva, E.A. Kotomin, and A.K. Dauletbekova, Ab initio calculations of MgF2 (001) AND (011) surfaces as well as bulk and surface F centers. Abstracts: B45.

A-304. R. Merkle, L. Wang, Yu.A. Mastrikov, E.A. Kotomin, and J. Maier, Mechanistic insight into oxygen exchange on mixed conducting oxides from experiments and theory. Abstracts of International conference on Functional materials and nanotechnologies, FMNT-2011 (Riga, Latvia, April, 2011). p. 13.

A-305. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M.M. Kuklja, D. Fuks, and J. Maier, First principles modeling of oxygen incorporation into oxygen permeation membranes and SOFC cathodes. Ibid., Abstracts, p. 18.

A-306. Yu.F. Zhukovskii, D. Bocharov, D. Gryaznov, and E.A. Kotomin, First-principles simulations on initial stage of uranium nitride surface oxidation.Ibid., Abstracts, p. 20.

A-307. E. Blokhin, D. Gryaznov, E.A. Kotomin, R.A. Evarestov, and J. Maier, Phonon calculations in perfect and defective SrTiO3 perovskites. Ibid., Abstracts, p. 65.

A-309. A.F. Fix, R.I. Eglitis, E.A. Kotomin, A.K. Dauletbekova, and F.U. Abuova, Ab initio calculations of bulk and surface F centers in MgF2. Ibid., Abstracts, p. 158

A-310. A. Sorokin, Yu.F. Zhukovskii, J. Purans, and E.A. Kotomin, Influence of Al and Ga dopants on electronic properties of ZnO: ab initio simulations. Ibid., Abstracts, p. 164.

A-311. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, and A. Moeslang, Ab initio calculations of pair-wise interactions between defects for ODS steels. Ibid., Abstracts, p. 165.

A-312. D. Bocharov, Yu.F. Zhukovskii, D. Gryaznov, and E.A. Kotomin, UN (110) surface properties: ab initio calculations. Ibid., Abstracts, p. 166.

A-313. D. Gryaznov, E. Heifets, and E.A. Kotomin, Density functional theory calculations on magnetic properties of actinide compounds. Ibid., Abstracts, p. 167.

A-314. E.A. Kotomin, D. Gryaznov, R.A. Evarestov, V.E. Alexandrov, and J. Maier, Confinement effects for ionic carriers in perovskite ultrathin films. Abstracts of Spring European Materials Research Society (E-MRS) Meeting (Nice, France, May, 2011). Abstracts CL-4.

A-315. Yu.N. Shunin, Yu.F. Zhukovskii, N. Burlutskaya, and S. Bellucci, Electric properties of junctions between 1D carbon nanostructures and metal substrate: theoretical simulations. Ibid., Abstract EP-8.

A-316. V. Pankratov, A.I. Popov, and E.A. Kotomin, Polarons in complex oxides. Ibid., Abstract LP-15.

A-317. A.I. Popov, E.A. Kotomin, V. Pankratov, and J. Maier, Generalization of Rabin-Klick diagram for a whole family of alkali halides. Ibid., Abstract LP-16.

A-318. L. Petit, A. Svane, E.A. Kotomin, and D. Gryaznov, First-principles calculations of the electronic and atomic structures of radiation defects in PuO2. Ibid., Abstract L6-2.

A-319. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, V.A. Borodin, E. A. Kotomin, and A. Moeslang, Modelling of interactions between Y, O and vacancy clusters in fcc Fe lattice. Ibid., Abstract VP-7.

A-320. D. Bocharov, Yu.F. Zhukovskii, D. Gryaznov, and E.A. Kotomin, First-principles simulations on initial stages of UN(001) surface oxidation. Ibid., Abstract V4-17.

A-321. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M.M. Kuklja, D. Fuks, S.N. Rashkeev, and J. Maier, First-principles modeling of oxygen incorporation into SOFC cathode and permeation membranes. ibid., Abstract X13-5.

A-322. E.A. Kotomin, R. Merkle, J. Maier, Yu. Mastrikov, and M.M. Kuklja, First-principles simulations of oxygen defects in reducible perovskites. CECAM workshop on Understanding Structure and Functions of Reducible Oxide Systems (Zaragoza, Spain, June, 2011). Abstracts, p. 38

A-323. Yu.A. Mastrikov, Yu.F. Zhukovskii, E.A. Kotomin, P.V. Vladimirov, and A. Moeslang, Models of point defects in bcc-Fe lattice for simulation of ODS nanocluster. Abstracts of Annual Monitory Meeting of European Fusion Development Agreement, EFDA - 2011 (Frascati, Italy, June, 2011).

A-324. R. Merkle, L. Wang, Yu. Mastrikov, E.A. Kotomin, and J. Maier, Mechanistic insight into oxygen exchange on mixed conducting oxides from experiments and theory. International Symposium on Reactivity of Solids (Bordeaux, France, June-July, 2011).Abstract O2.

A-325. E.A. Kotomin, R. Merkle, Yu.A. Matrikov, M.M. Kuklja, and J. Maier, First princliples modeling of oxygen vacancy formation and mobility in (Ba,Sr)(Co,Fe)O3 perovskites. 18th International Conference on Solid State Ionics (Warsaw, Poland, July, 2011), Abstracts, p.28.

A-326. D. Bocharov, Yu.F. Zhukovskii, D. Gryaznov, and E.A. Kotomin, A comparative study of the UN (100) and (110) surfaces: first principles DFT calculations. School on Synergy between modelling and experiments for the investigation of nuclear fuels. (Cambridge, UK, September, 2011).

A-327. A. Weizman, D. Fuks, E.A. Kotomin, and J. Maier, Ab-initio thermodynamic analysis of the (La,Sr)CoO3 solid solutions. European Congress on Advanced Materials and Processes, EUROMAT-2011 (Montpellier, France, September, 2011).

A-328. E.A. Kotomin, D. Gryaznov, L. Petit, and A. Svane, First principles calculations of the electronic and atomic structure of radiation defects in PuO2. Materials Science and Technology, MST-2011 (Columbus, Ohio, USA, October, 2011).Abstracts: p. 97.

A-329. E.A. Kotomin, D. Gryaznov, E. Blokhin, R.A. Evarestov, V. Alexandrov, and J. Maier, Confinement effects for ionic carriers in SrTiO3 ultrathin films. Ibid., Abstracts: p. 61.

A-330. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M.M. Kuklja, and J. Maier, First principles calculations of oxygen incorporation into SOFC cathode materials. Ibid., Abstracts: p. 89.

A-331. D. Gryaznov, R.A. Evarestov, E. Blokhin, E.A. Kotomin, and J. Maier, Ab initio thermodynamic calculations of oxygen vacancies in perovskites: the case study of (La,Sr)(Co,Fe)O3 and SrTiO3. 8th International Conference Functional Materials and Nanotechnologies– FMNT-2012 (Riga, Latvia, April, 2012).- Abstract: p. 67.

A-332. J.R. Kalnin and E.A. Kotomin, One-dimensional diffusion in heterogeneous medium. Ibid, Abstracts, p. 68.

A-333. E.A. Kotomin, Yu.A. Mastrikov, J. Maier, M.M. Kuklja, A. Weizman, and D. Fuks, First principles calculations of structural stability for complex perovskites. Ibid., Abstracts, p. 71.

A-334. Yu.A. Mastrikov, D. Gryaznov, E.A. Kotomin, R. Merkle, M.M. Kuklja, and J. Maier, First principles study of oxygen vacancies in perovskite solid solutions. Ibid., Abstracts, p. 81.

A-335. G. Zvejnieks, V.N. Kuzovkov, E.A. Kotomin, and M.O. de la Cruz, Microscopic approach to the kinetics of pattern formation of charged molecules on surfaces. Ibid., Abstracts, p. 99.

A-336. E. Blokhin, D. Gryaznov, R.A. Evarestov, and J. Maier, A new approach to the engineering of ab initio materials simulations on an example of CRYSTAL, VASP and

WIEN-2k packages. Ibid., Abstracts, p. 115.

A-337. E. Blokhin, A. Kuzmin, J. Purans, E.A. Kotomin, R.A. Evarestov, and J. Maier, Joint theoretical-experimental study of iron impurities and oxygen vacancies in SrTiO3. Ibid., Abstracts, p. 116.

A-338. A. Sorokin, D. Gryaznov, Yu.F. Zhukovskii, E.A. Kotomin, and J. Purans, First principles calculations of defective ZnO crystals: the role of symmetry and phonons. Ibid., Abstracts, p. 126.

A-339. A. Usseinov, A. Sorokin, Yu.F. Zhukovskii, E.A. Kotomin, A.T. Alikbekov, and J. Purans, Ab initio calculations of hydrogen impurities in ZnO. Ibid., Abstracts, p. 127.

A-340. P. Merzlakov, G. Zvejnieks, V.N. Kuzovkov, E.A. Kotomin, K.D. Li, and L.M. Wang, Analysis of void superlattice formation in CaF2. Ibid., Abstracts, p. 282.

A-341. G. Zvejnieks, V.N. Kuzovkov, and E.A. Kotomin, Atomistic theory of mesoscopic pattern formation induced by bimolecular surface reactions between oppositely charged molecules. Ibid., Abstracts, p. 283.

A-342. V.N. Kuzovkov, E.A. Kotomin, and M.O. de la Cruz, The non-equilibrium charge screening effects in diffusion-driven systems. Ibid., Abstracts, p. 285.

A-343. D. Bocharov, Yu.F. Zhukovskii, D. Gryaznov, and E.A. Kotomin, Ab initio modeling of uranium nitride grain boundary interfaces. Ibid., Abstracts, p. 304.

A-344. F.U. Abuova, A.F. Fix, A.T. Akilbekov, S. Piskunov, E.A. Kotomin, and R.I. Eglitis, Ab initio calculations of bulk and surface defects in MgF2 crystals. Ibid., Abstracts, p. 305.

A-345. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, and A. Moeslang, Quantum chemical simulations on binding energies of pair and tripe-wise defects in fcc-Fe lattice for ODS steels. Ibid., Abstracts, p. 306.

A-346. F.U. Abuova, A.F. Fix, A.T. Akilbekov, E.A. Kotomin, and R.I. Eglitis, Ab initio calculations of bulk and surface color centers in MgF2 crystals. 13th International V.A. Fock Meeting on Quantum and Computational Chemistry (Astana, Kazakhstan, April, 2012). Abstract: p. 48.

A-347. Yu.F. Zhukovskii, D. Bocharov, D. Gryaznov and E.A.Kotomin, First-principles simulations on surface properties and oxidation of uranium mononitrde. Ibid., Abstract: p. 53.

A-348. Yu.A. Mastrikov, E.A. Kotomin, R. Merkle, M.M. Kuklja, and J. Maier, First principles calculations of formation and migration of oxygen vacancies in La1-xSrxCo1-yFeyO3 perovskites. VII. Spring European Materials Research Society (E-MRS) Meeting (Strasbourg, France, May, 2012). Abstract: C7-2.

A-349. M.M. Kuklja, Yu.A. Mastrikov, B. Jansang, and E.A. Kotomin, First principles calculations of (Ba,Sr)(Co,Fe)O3 structural stability. Ibid., Abstract: C7-3.

A-350. A. Weizman, D. Fuks, D. Gryaznov, and E.A. Kotomin, Ab initio study of phase competition in (Lax,Sr1-x)CoO3. Ibid., Abstract CP5-8.

A-351. D. Gryaznov, E. Heifets, and E.A. Kotomin, The first-principles treatment of the electron-correlation and spin-orbital effects in uranium mononitride nuclear fuels. Ibid., Abstract: E1-4.

A-352. E.A. Kotomin, D. Gryaznov, D. Bocharov, and Yu.F. Zhukovskii, Ab initio simulations of oxygen adsorption and migration upon uranium nitride surfaces. Ibid., Abstract: E2-2.

A-353. Yu.A. Mastrikov, P.V. Vladimirov, V.A. Borodin, Yu.F. Zhukovskii, E.A. Kotomin, and A. Moeslang, Ab initio simulation of growth of vacancies formed clusters in gamma-Fe lattice. Annual Monitory Meeting of European Fusion Development Agreement, EFDA - 2012 (Ljubljana, Slovenia, June, 2012).

A-354. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M. Kuklja, D. Fuks, and J. Maier, First principles calculations on defects in ABO3 perovskites: Applications for oxygen permeation membranes and SOFC cathodes. 17th International Conference on Defects in Insulating Materials, ICDIM-2012 (Santa Fe, Arizona, USA, June, 2012). p.18.

A-355. F.U. Abuova, A.K. Dauletbekova, A.T. Akilbekov, E.A. Kotomin, and Zh.K. Yermekova, First principles calculations on radiation defects in MgF2 crystals. Ibid., p.110.

A-356. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M. Kuklja, D. Fuks, and J. Maier, Ab initio modelling of oxygen transport in mixed conducting perovskites. 10th International Symposium on Systems with fast ionic transport (ISSFIT), 1-4 July, 2012, Chernogolovka, Russia, p.14.

A-357. A. Weizman, D. Fuks, D. Gryaznov, and E.A. Kotomin, Ab initio study of phase equilibria in (Lax,Sr1-x)CoO3 solid solutions. The 15th Israel Materials Engineering Conference (IMEC-15), (Dead Sea, Israel, February-March, 2012).

A-358. R. Merkle, L. Wang, Y. A. Mastrikov, E. A. Kotomin, and J. Maier, Oxigen exchange kinetics on perovskite surfaces: importance of electronic and ionic defects. Nature Materials: Frontiers in Electronic Materials: Correlation Effects and Memristive Phenomena (Aachen, Germany, June, 2012).

A-359. D. Fuks, E.A. Kotomin, A. Weizman, Yu.A. Mastrikov, M.M. Kuklja, and J. Maier, Ab initio thermodynamic study of phase competition in ABO3-type multicomponent solid solutions. E-MRS 2011 Fall Meeting (Warsaw, Poland, September, 2012). Abstract C-XI-2.

A-360. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M.M. Kuklja, D. Fuks, and J. Maier, First principles calculations of defects in ABO3 perovskites: applications for oxygen permeation membranes and SOFC cathodes. Ibid., Abstract C-XI-3.

A-361. E. Blokhin, E.A. Kotomin, D. Gryaznov, R.A. Evarestov, and J. Maier, Confinement effects for point defects in perovskite ultrathin films. Abstract I-I-5.

A-362. M.M. Kuklja, D. Fuks, O. Sharia, Yu.A. Mastrikov, and E.A. Kotomin, Vacancy-stabilized complex perovskites for SOFC applications. Ibid., Abstract L-VII-2.

A-363. A. Weizman, D. Fuks, D. Gryaznov, E.A. Kotomin, Ab initio study of phase transformations in $(La_x,Sr_{1-x})CoO_3$: Beyond regular solid solutions. 14th International

IUPAC Conference on High Temperature Materials Chemistry, HTMC-14 (Beijing, China, September, 2012).

A-364. F.U. Abuova, A.B. Useinov, A.T. Akilbekov, E.A. Kotomin, S.Piskunov, First-principles calculations of radiation defects in magnesium fluorite, 15th International Conference of Radiation Physics and Chemistry of Condensed Matter (Tomsk, Russia, September, 2012). Abstracts, p.8-9.

A-365. R. Merkle, L. Wang, A. Wedig, Yu.A. Mastrikov, E.A. Kotomin, and J. Maier, Oxygen exchange kinetics on solid oxide fuel cell cathode materials - mechanistic interpretation and the importance of defects. Fall MRS Meeting (Boston, USA, November, 2012). Abstract I1.05

A-366. M. Kuklja, E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, and J. Maier, Comparative analysis of oxygen vacancy diffusion in LSCF and BSCF perovskite solid solutions: Ab initio modeling. ibid., Abstract I9.17.

A-367. M. Kuklja, D. Fuks, O. Sharia, Yu.A. Mastrikov, and E.A. Kotomin, Degradation and stability of complex perovskites for energy applications. Ibid., Abstract I2.02.

A-368. G. Zvejnieks, P. Merzlyakov, V.N. Kuzovkov, and E.A. Kotomin, Cellular automata modeling of void lattice self-organization in CaF2 under irradiation. IV. 9th International Conference "Functional Materials and Nanotechnologies" FM-NT-2013 (Tartu, Estonia, April, 2013). Abstract: OR-29.

A-369. Yu.F. Zhukovskii, A. Gopejenko, Yu.A. Mastrikov, E.A. Kotomin, P.V. Vladimirov, and A. Moeslang, Modeling of Y-O precipitation in bcc-Fe and fcc-Fe lattices. Ibid., Abstract: OR-35.

A-370. E.A. Kotomin, M.M. Kuklja, Yu.A. Mastrikov, O. Sharia, D. Fuks, and J. Maier, Prediction of structural stability of complex perovskites for solid oxide fuel cells from first principles. Ibid., Abstract: OR-36.

A-371. P. Merzlyakov, G. Zvejnieks, V.N. Kuzovkov, and E.A. Kotomin, Statistical analysis of void lattice formation in CaF2. Ibid., Abstract: PO-30.

A-372. F.U. Abuova, A.T. ?kilbekov, E.A. ??t?min, and S. Piskunov, First-principles calculations of defects in MgF2. Ibid., Abstract: PO-146.

A-373. A. Usseinov, E.A. Kotomin, Yu.F. Zhukovskii, J. Purans, A. Sorokin, and A.T. Akilbekov, First-principles calculations of ZnO crystals doped with hydrogen. Ibid., Abstract: PO-168.

A-374. A. Sorokin, D. Gryaznov, E.A. Kotomin, and J. Purans, First-principles calculations of electronic structure and phonon properties of Al- and H-doped ZnO.Ibid., Abstract: PO-169.

A-375. E.A. Kotomin, R. Merkle, Yu. Mastrikov, M.M. Kuklja, D. Fuks, J. Maier. Ab initio modeling of oxygen transport in mixed conducting perovskites for SOFC applications. – 2013 MRS spring meeting (San Francisco), Symp. G, Abstract G6.02 (p.157)

A-376. E.A. Kotomin, E. Blokhin, D. Gryaznov, R.A.Evarestov, and J. Maier, Ab initio study of confinement effects for ionic carriers in perovskite ultrathin films. –Ibid., symp. XX, Abstract XX1.05 (p.386).

A-377. E.A. Kotomin, M.M. Kuklja, D. Fuks, Yu. A. Mastrikov, O.Sharia, J. Maier. Understanding structural stability of complex perovskites for solid oxide fuel cells: First principles calculations.– E-MRS 2013 Spring Meeting, symposium F : Nanomaterials for energy conversion and storage, Strasbourg, France (May 27-31, 2013). –Abstract F.P2-1.

A-378. E.A. Kotomin, D. Bocharov, D. Gryaznov, and Yu.F. Zhukovskii. Ab initio simulations of oxygen interaction with surfaces, interfaces and grain boundaries in uranium mononitride nuclear fuels Ibid., symposium M : Basic research on ionic-covalent materials for nuclear applications, Abstract M 7-2.

A-379. V.N. Kuzovkov, G. Zvejnieks, E.A. Kotomin. Non-equilibrium charge screening in pattern formation kinetics for oppositely charged nanoparticles Ibid., symposium N : Atomic-scale engineering of multifunctional nano-sized materials and films, Abstract N. P1-10.

A-380. G.Zvejnieks, V.N. Kuzovkov, E.A. Kotomin. Characterization of self-assembled charged nanoparticle structures. – Ibid., symp. N, Abstract N.P1-9.

A-381. D. Gryaznov, E.A. Kotomin, E. Blokhin, R.A. Evarestov, J. Maier, J. Purans. A comparative ab initio thermodynamic study of oxygen vacancies in oxides. Ibid., symp. O, Abstract O.P2-5

A-382. A. Useinov, E.A. Kotomin, Yu. Zhukovskii, J. Purans, A. Sorokin, A. Akilbekov. Atomic and electronic structure of hydrogen-doped ZnO: Ab initio hybrid calculations. Ibid., Abstract O.P2.-6.

A-383. E.A. Kotomin, Yu. Mastrikov. Ab initio Modelling of Oxygen Transport in (Ba,Sr)(Co,Fe)O_3 Perovskite Solid Solutions for Solid Oxide Fuel Cells. WP4 meeting of the EC COST CM 1104 "Reducible oxides" (London, UK, May 9-10, 2013). Abstracts, p.1.

A-384. Yu. Mastrikov, E.A. Kotomin. Ab initio modeling of oxygen reduction and diffusion in perovskite solid solutions for SOFC and permeation membranes. – Ibid., p.3.

A-385. Gryaznov D, Kotomin EA, Bussmann-Holder A, Maier J. A comparative ab initio thermodynamic study of oxygen vacancies in oxide perovskites: role of phonons. — International Symposium on Recent Electronic-Structure Theories and Related Experiments, June 12 -15, 2013, Max Planck Institute for Solid State Research, Stuttgart, Germany. Poster 33.

A-386. Kotomin E, Mastrikov YuA, Merkle R, Maier J. A comparative analysis of oxygen vacancy diffusion in LSCF and BSCF perovskite solid solutions: ab initio modeling. — Ibid., poster 16.

A-387. Merkle R., Mastrikov Yu., Kotomin E.A., Kuklja M.M., Maier J. Comparative analysis of oxygen mobility in (La,Sr)(Co,Fe)O_3 perovskites based on ab initio modeling. – Bunsentagung 2013 meeting [Annual meeting of German Physical Chemistry Socienty] (Karlsruhe, Germany, May 9-11). –Abstracts, paper 1188.

A-388. Merkle R., Wang L., Mastrikov Yu., Kotomin E.A., Kuklja M.M., Maier J. Oxygen exchange mechanism on mixed conducting perovskites: insight from experiment and theory.– 10th symposium on fuell cell and battery modelling and experimental validation (ModVal-10) (Bad Boll, Germany, March 19-20, 2013). Abstracts, p.37.

A-389. Kuklja M.M., Mastrikov Yu., Merkle R., Kotomin E.A., Maier J. Comparative analysis of oxygen mobility in LSCF. – International symposium on Solid State Ionics (SSI-19) (Kyoto, Japan, June 3-7, 2013).– Abstract A2-08.

A-390. Merkle R., Wang L., Wedig A., Mastrikov Yu., Kotomin E.A., Maier J. Oxygen exchange kinetics on SOFC cathode materials – reaction mechanism and importance of defects.– Ibid., Abstract C1-12.

A-391. Yu.A. Mastrikov, P.V. Vladimirov, V.A. Borodin, Yu.F. Zhukovskii, E.A. Kotomin, and A. Moeslang. Ab initio modeling of nY/nVFe complexes diffusion in the Fe lattice. –Annual Monitory Meeting of European Fusion Development Agreement, EFDA - 2013 (Bucharest, Romania, June, 2013).

A-392. M.M. Kuklja, E.A. Kotomin, O. Sharia, Yu.A. Mastrikov, and J. Maier. Radiation defects in complex solid solutions. 17th International Conference on Radiation Effects in Insulators, REI'17 (Helsinki, Finland, July, 2013). Abstract: O-33.

A-393. F.U. Abuova, A.T. Akilbekov, E.A. Kotomin, S. Piskunov, and V.M. Lisitsyn. Ab initio modelling of radiation damage in MgF2. - Ibid., Abstract PB-13.

A-394. D. Gryaznov, E.A. Kotomin, E. Blokhin, R.A. Evarestov, J. Maier, and J.Purans. A comparative ab initio thermodynamic study of oxygen vacancies in oxides.- Ibid., Abstract: PB-18.

A-395. E.A. Kotomin, Yu.A. Mastrikov, R. Merkle, and J. Maier. Ab initio modelling of oxygen reduction and transport in perovskites for solid oxide fuel cells. - Workshop on New Horizons in Electrochemistry- at the Boundary to Physics and Materials Science (Capri, Italy, August, 2013). Abstract: p. 24.

A-396. E.A. Kotomin, First principles modelling of strongly non-stoichiometric perovskite solid solutions. – Advances in the Chemistry of Disordered Solids: Workshop Honouring the Contributions of Professor Patrick Jacobs to Solid State Chemistry (London, UK, September, 2013).

A-397. M. Kuklja, E.A. Kotomin, D. Fuks, Yu.A. Mastrikov, O. Sharia, R. Merkle, and J. Maier. First principles modeling of complex perovskites for energy applications. 246th American Chemical Society National Meeting and Exposition (Indianapolis, USA, September, 2013). Abstracts: p. 416.

A-398. D. Fuks, M.M. Kuklja, Yu.A. Mastrikov, and E.A. Kotomin. Phase stability versus decomposition in complex perovskite solid solutions from DFT study. — European Congress on Advanced Materials and Processes, EUROMAT 2013 (Sevilla, Spain, September, 2013). Symposium E1.III. Materials for Fuel Cells.

A-399. A. Usseinov, E.A. Kotomin, Yu.F. Zhukovskii, J. Purans, A.T. Akilbekov, and A.K. Dauletbekova. Hydrogen adsorption on non-polar surfaces of ZnO: Ab initio calculations. 6th International Conference Physics of Disordered Systems (Lviv, Ukraine, October, 2013). - Abstracts: p. 91.

A-400. Yu.A. Mastrikov and E.A. Kotomin. First principles modeling of processes in complex perovskites for solid oxide fuel cells. - 2nd General COST Meeting, Action CM 1104 "Reducible Oxide Chemistry" (Uppsala, Sweden, November, 2013). Abstracts, p. 67.

A-401. E.A. Kotomin, D. Fuks, M. Kuklja, Yu.A. Mastrikov, R. Merkle and J. Maier, "Ab initio modelling of pervoskite solid solutions for solid oxide fuel cells and permeation membranes". — 16th Israel Materials Engineering Conference, (Haifa, Israel, February, 2014). Abstracts, p. 26.

A-402. E.A. Kotomin and D. Gryaznov, "Ab initio modelling of a role of Sr doping in permeation membranes". — III. Workshop on Permeation membranes (GREEN-OTM EC Project meeting), (Valencia, Spain, March-April, 2014).

A-403. Yu.A. Mastrikov, M.M. Kuklja, R. Merkle, E.A. Kotomin, and J. Maier, "Oxygen Mobility in LSCF and BSCF Perovskites from ab Initio Modeling". Materials Research Society, Spring Meeting, (San Francisco, USA, April, 2014). Abstract: L8.02.

A-404. D. Gryaznov, J. Begens, and E.A. Kotomin, First principles calculations on oxygen vacancy behaviour in Sr-doped complex perovskites for permeation membranes and solid oxide fuel cells. WG4 COST Meeting, Action CM 1104 "Reducible Oxide Chemistry" (Riga, Latvia, April, 2014). Abstracts: p. 23.

A-405. Yu.A. Mastrikov and E.A. Kotomin, "First-principles modelling of oxygen transport in complex perovskites". Ibid., p. 29.

A-406. A.I. Popov, A.Ch. Lushchik, Ch.B. Lushchik, and E.A. Kotomin, Analysis of excitonic mechanism of defect formation in insulating materials: Generalization of Rabin-Klick diagram for a whole family of alkali halides. Ibid., p. 30.

A-407. E.A. Kotomin, M.M. Kuklja, D. Fuks, Yu.A. Mastrikov, and J. Maier, A comparative study of structural stability of complex perovskites for solid oxide fuel cells: First principles thermodynamic calculations. Euro-MRS 2014 Spring Meeting (Lille, France, May, 2013). Abstract: C.4.4.

A-408. A.U. Abuova, T.M. Inerbaev, A.T. Akilbekov, Yu.A. Mastrikov, and E.A. Kotomin, First principles modeling of Ag adsorption on the MnO2- and LaO-terminated surfaces of LaMnO3(001) Ibid., C/P1.1.

A-409. G. Kaptagai, T.M. Inerbaev, A.T. Akilbekov, Yu.A. Mastrikov, and E.A. Kotomin, Water interaction with fluorine-doped Co3O4 (100) and (111) surfaces. Ibid., C/P1.10.

A-410. Yu.A. Mastrikov, E.A. Kotomin, R. Merkle, M.M. Kuklja, and J. Maier, First principles calculations of formation and migration of oxygen vacancies in the bulk and at the surface of complex perovskites for solid oxide fuel cell cathodes Ibid., Abstract: C/P1.11.

A-411. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M.M. Kuklja, and J. Maier, Ab initio modeling of oxygen reduction reaction in mixed conducting perovsites for solid oxide fuel cells. Ibid., Abstract: CC.1.6.

A-412. M. Arrigoni, D. Gryaznov, E.A. Kotomin, and J. Maier, Confinement effects for ionic carriers in ABO3 perovskite ultrathin films. Ibid., EO.5.3.

A-413. Yu.A. Mastrikov, P.V. Vladimirov, V.A. Borodin, A. Gopejenko, Yu.F. Zhukovskii, E.A. Kotomin, and A. Moeslang, Ab initio simulation of the initial steps of the ODS particle formation process in bcc iron matrix. Ibid., EP.2.73.

A-414. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M.M. Kuklja, and J. Maier, "Ab initio modelling of oxygen reduction reaction in mixed conducting pervoskites for solid oxide fuell cells". - International Symposium on Reactivity of Solids, (St.Petersburg, Russia, June, 2014). Abstract: p. 99.

A-415. V.N. Kuzovkov, M. Olvera de la Cruz, G. Zvejnieks, and E.A. Kotomin, "Diffusion and self-assembly of charged nanoparticles in three-dimensional condensed systems". — DSL2014 conference (Paris, France, June, 2014). Abstracts: p. 214.

A-416. E.A. Kotomin, Yu. Mastrikov, and M. Kuklja, "Structural instability of perovskite solid solutions". Electrochemistry workshop (Asilomar, USA, July, 2014).

A-417. T. Bjorheim, E.A. Kotomin, R. Haugsrud, and J. Maier, "Defect thermodynamics of BaZrO3 from first principles phonon calculations". — International conference on solid state protonic conductors (SSPC-17) (Seoul, Korea, September, 2014).

A-418. D. Gryaznov, D. Bocharov, E.A. Kotomin, and Yu.F Zhukovskii, "Ab initio simulations of oxygen interaction with surfaces and interfaces in uranium mononitride". — Euro-MRS Fall Meeting, (Warsaw, Poland, September, 2014). Abstracts: G9.44.

A-419. E.A. Kotomin, R. Merkle, Yu. Mastrikov, M.M. Kuklja, and J. Maier, "First principles calculations of oxygen transport in SOFC cathode materials". — Materials Science and Technology (MST-14) (Pittsburgh, USA, October, 2014). Abstracts, p.53.

A-420. M.M. Kuklja, E.A. Kotomin, D. Fuks, Yu. Mastrikov, and O. Sharia, "Disorder and structural stability of complex perovskites for solid oxide fuel cells: ab initio modeling". Ibid., Abstracts, p. 103.

A-421. E.A. Kotomin, M. Arrigoni, D. Gryaznov, T. Bjorheim, and J. Maier, "Confinement effects for ionic carriers in BaZrO3 ultrathin films". Ibid., Abstracts, p. 148.

A-422. R. Merkle, D. Poetzsch, D. Gryaznov, E.A. Kotomin, and J. Maier, Mixed conducting perovskites as solid oxide fuel cell cathode materials: Insight from experiments and theory. — Joint 12th RCBJCF Symposium and 9th FMNT Conference (Riga, Latvia, September-October, 2014). Abstracts: p. 75.

A-423. T.S. Bjorheim, R. Haugsrud, J. Maier, and E.A. Kotomin, Defect thermodynamics of BaZrO3 from first principles phonon calculations. Ibid., Abstracts: p. 237.

A-424. E.A. Kotomin, M.M. Kuklja, Yu.A. Mastrikov, R. Merkle, and J. Maier, Challenges in energy applications of non-stoichiometric complex perovskites. Ibid., Abstracts: p. 247.

A-425. A.U. Abuova, T.M. Inerbaev, E.A. Kotomin, A.T. Akilbekov, and Yu.A. Mastrikov, Ab Initio modelling of Ag adsorption on the MnO2- and LaO-terminated LMO(001) surfaces. Ibid., Abstracts: p. 271.

A-426. A. Usseinov, E.A. Kotomin, Yu.F. Zhukovskii, J. Purans, A.T. Akilbekov, and A.K. Dauletbekova, Electronic effects on hydrogen-adsorbed surfaces of ZnO: First principles study. Ibid., Abstracts: p. 275.

A-427. A. Platonenko, S. Piskunov, Yu.F. Zhukovskii, and E.A. Kotomin, Ab initio simulations on Frenkel pairs of radiation defects in corundum. Ibid., Abstracts: p. 278.

A-427. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, Yu.A. Mastrikov, V.A. Borodin, and A. Moeslang, Ab initio calculations of interactions between Y and O impurity atoms and vacancies in bcc- and fcc-iron lattices. Ibid., Abstracts: p. 282.

A-428. A.I. Popov, A.Ch. Lushchik, Ch.B. Lushchik, and E.A. Kotomin, Analysis of excitonic mechanism of defect formation in insulating materials: Generalization of Rabin-Klick diagram for a whole family of alkali halides. Ibid., Abstracts: p. 333.

A-429. G. Kaptagay, T.M. Inerbaev, E.A. Kotomin, A.T. Akilbekov, Yu.A. Mastrikov, and F.U. Abuova, Research of interaction fluorine-doped Co3O4 (100) and (111) surfaces with water. Ibid., Abstracts: p. 340.

A-430. E.A. Kotomin, R. Merkle, Yu. Mastrikov, M.M. Kuklja, and J. Maier, First principles calculations of oxygen transport in SOFC cathode materials. – Abstracts of 18.meeting on Materials Science and Technology (MST-14) (Pittsburgh, USA, October, 2014). p.53.

A-431. M.M. Kuklja, E.A. Kotomin, D. Fuks, Yu. Mastrikov, and O. Sharia, "Disorder and structural stability of complex perovskites for solid oxide fuel cells: ab initio modeling", Ibid. p. 103.

A-432. E.A. Kotomin, M. Arrigoni, D. Gryaznov, T. Bjorheim, and J. Maier, "Confinement effects for ionic carriers in BaZrO3 ultrathin films". Ibid., p. 148.

A-433. E.A. Kotomin, "Computer modeling of new materials from first principles". Abstracts of the International conference on Atomistic Simulations of Functional Materials (Moscow, Russia, December, 2014).

A-434. G. Kaptagai, T.M. Inerbaev, A.T. Akilbekov, Yu.A. Mastrikov, and E.A. Kotomin, Theoretical modeling of water adsorption on the fluorine-doped Co3O4 (111) surface. Abstract B/P2.23 at EMRS spring meeting (Lille, France, May 2015).

A-435. Yu.F. Zhukovskii, A. Platonenko, S. Piskunov, and E.A. Kotomin, Ab initio computer simulations of radiation defects in corundum. Ibid., Abstract: G.2.2.

A-436. V.M. Lisitsyn, L.A. Lisitsyna, E.A. Kotomin, A.I. Popov, and J. Maier, The peculiarities of the excitonic mechanism of defect formation and stabilisation in fluorides. Ibid., Abstract: G.2.3.

A-437. V.N. Kuzovkov, E.A. Kotomin, A.I. Popov, and R. Vila, Kinetics of radiation-induced colloid formation in Al2O3 and NaCl crystals. Ibid., Abstract: G.6.4.

A-438. Yu.A. Mastrikov, P.V. Vladimirov, V.A. Borodin, A. Gopejenko, Yu.F. Zhukovskii, E.A. Kotomin, and A. Moeslang, Interaction of yttrium and oxygen with vacancy clusters within bcc-Fe matrix. Ibid., Abstract: G/P.11.

A-439. A.I. Popov, E.A. Kotomin, and J. Maier, Analysis of the self-trapped hole center mobility and recombination in alkali halides and complex metal halides. Ibid., Abstract: G/P.20.

A-440. M. Arrigoni, T.S. Bjoerheim, E.A. Kotomin, and J. Maier, First principles thermodynamics of oxygen vacancies in ultrathin films of BaZrO3. Ibid., Abstract: M.11.3.

A-441. E. Heifets, E.A. Kotomin, R. Merkle, and J. Maier, Ab initio study of BiFeO3 stability. Ibid., Abstract: M/P.13.

A-442. Yu.A. Mastrikov, E.A. Kotomin, R. Merkle, M.M. Kuklja, and J. Maier, Ab initio modelling of oxygen vacancies formation and migration in the bulk and on the surface of complex perovskites for solid oxide fuel cell cathodes. Ibid., Abstract: M/P.31.

A-443. A.U. Abuova, E.A. Kotomin, Yu. A. Mastrikov, T.M. Inerbaev, and A.T. Akilbekov, LaMnO3 (001) surface doping with Ag and its catalytic effect on the oxygen reduction. Abstract: N/P1.9.

A-444. A. Usseinov, E.A. Kotomin, A.T. Akilbekov, Yu.F. Zhukovskii, J. Purans, and F. Abuova, Hydrogen migration and stability in ZnO: Ab initio calculations. Abstract: N/P2.27.

A-445. E.A. Kotomin, M.M. Kuklja, D. Fuks, Yu.A. Mastrikov, and J. Maier, Structural stability of complex perovskites for solid oxide fuel cells from first principles calculations. Abstract: N/P2.35.

A-445. E.A. Kotomin, " Defects and stability of non-stoichiometric complex perovskites". – Invited talk at Leoben University, Austria, 20. March 2015.

A-446. T.S.Bjoerheim, E.A. Kotomin, and J. Maier, "Defect chemistry of CeO2 surfaces from first principles and space charge theory"–227th Electrochemical Society Meeting (Chicago, USA, May, 2015). - Abstract: 1775.

A-447. E.A. Kotomin, Yu.A. Mastrikov, R. Merkle, M.M. Kuklja, and J. Maier, "First principles calculations of formation and migration of oxygen vacancies in the bulk and on surface of complex perovskites for solid oxide fuel cell cathodes". – 20th International conference on Solid State Ionics (Keystone Colorado, USA, June, 2015). Abstract: D4.04.

A-448. T.S. Bjorheim, E.A. Kotomin, and J. Maier, "Defect chemistry of CeO2 surfaces from first principles and space charge theory". Ibid., Abstract: D8.07.

A-449. M.M. Kuklja, E.A. Kotomin, D. Fuks, Yu.A. Mastrikov, and J. Maier, "Structural stability of complex perovskites for solid oxide fuel cells from first principles calculations". Ibid., Abstract: A2.01.

A-450. M. Arrigoni, E.A. Kotomin, J. Maier and T.S. Bjorheim, "First principles thermodynamics of oxygen vacancies in ultrathin films of BaZrO3". Ibid., Abstract: A2.04.

A-451. V.N. Kuzovkov and E.A. Kotomin, "Static and dynamic screening effects in diffusion-controlled self-assembly of charged nanoparticles". — 11th International Conference on Diffusion in Solids and Liquids DSL-2015 (Munich, Germany, June, 2015). Abstract: p. 153.

A-452. D. Gryaznov, R. Merkle, and E.A. Kotomin, "Hybrid density-functional calculations on oxygen vacancy behaviour in complex perovskite oxides". – 28th International Conference on Defects in Semiconductors (Helsinki, Finland, July, 2015). Abstract: p.22.

A-453. J.R. Kalnins, E.A. Kotomin, and V.N. Kuzovkov, " Effective diffusion coefficient in one-dimensional heterogeneous solids: a comparison of continuous and discrete lattice models". — 6th International Conference Diffusion Fundamentals (Dresden, Germany, August, 2015). Abstract: p.27.

A-454. V.N. Kuzovkov, E.A. Kotomin, A.I. Popov, and R. Vila, " Diffusion-controlled kinetics of metallic colloid formation in irradiated Al2O3, MgO and NaCl crystals". Ibid., Abstract: p.30.

A-455. V.N. Kuzovkov, G. Zvejnieks, and E.A. Kotomin, " Diffusion and self-assembly of charged nanoparticles in polar media: a competition between short-range and long-range interactions". Abstract: p.31.

A-456. E.A. Kotomin, D. Gryaznov, and Yu.A. Mastrikov, "Defects in complex perovskites for electrochemical applications". Abstracts of XXII. Solid state electrochemistry workshop (Roggensburg, Germany, September, 2015).

A-457. D. Gryaznov, M. Arrigoni, E.A. Kotomin, and A.I. Popov, "Hybrid DFT calculations of the electronic and phonon properties of defects in perovskite oxides". — E-MRS 2015 Fall Meeting, Symposium J (Ferroic perovskites for advanced materials) (Warsaw, Poland, September, 2015). Abstract: J6.

A-458. E.A. Kotomin, "Ab initio calculations of defects in complex perovskites for energy applications". 3rd International School-Conference on Atomistic Simulations of Functional Materials (Moscow, Russia, October 2015).

A-459. M.M. Kuklja, E.A. Kotomin, D. Fuks, Yu.A. Mastrikov, and J. Maier, "Structural (in)stability of complex perovskites for solid oxide fuel cells: first principles calculations". — Workshop on Fundamental Physics of Ferroelectrics, (Washington, USA, 31 January -4 February, 2016), Abstract, p. 25.

A-460. E.A. Kotomin, Yu.A. Mastrikov, R. Merkle, M.M. Kuklja, and J. Maier, "First principles calculations of oxygen vacancies in the bulk and on the surface of complex perovskites for solid oxide fuel cell cathodes". Ibid., Abstracts, p.102.

A-461. M. Arrigoni, E.A. Kotomin, J. Maier, D. Gryaznov, and R.A. Evarestov, A comparative ab initio analysis of oxygen vacancies on CeO2(111) surfaces and in the bulk. - E-MRS 2016 Spring Meeting (Lille, France, 2-6 May, 2016). Abstract: BB.1.3.

A-462. A.I. Popov, E.A. Kotomin, V.N. Kuzovkov, A. Lushchik, V.M. Lisitsyn, A. Akilbekov, and J. Maier, Modelling of F center annealing kinetics in neutron- and electron-irradiated MgF2 and MgO crystals. Ibid., Abstract: BB.8.2.

A-463. Yu.A. Mastrikov, P.V. Vladimirov, V.A. Borodin, A. Gopejenko, Yu.F. Zhukovskii, E. A. Kotomin, and A. Moeslang, Ab initio modelling of nY/mO nanoclusters in bcc Fe lattic. Ibid., Abstract: BB.9.2.

A-464. A.I. Popov, E.A. Kotomin, V.N. Kuzovkov, A. Lushchik, E. Shablonin, and E. Vasilchenko, Comparison of the diffusion-controlled F center thermal annealing in neutron- and heavy-ion irradiated Al2O3 crystals. Abstract: BB.P1.6.

A-465. A. Platonenko, Yu.F. Zhukovskii, S. Piskunov, and E.A. Kotomin, Ab initio simulations of radiation-induced oxygen defects in corundum. Ibid., Abstract: BB.P1.8.

A-466. Yu.A. Mastrikov, R. Merkle, E.A. Kotomin, M.M. Kuklja, and J. Maier, Effect of (La,Sr)MnO3 (001) surface terminations on oxygen reduction reaction rate Abstract: D.1.3.

A-467. D. Gryaznov, R. Merkle, E. A. Kotomin, and J. Maier,First principles calculations of protonic defects in La1-xSrxFeO3-delta perovskites Abstract: D.3.3.

A-468. E.A. Kotomin, M. Arrigoni, J. Maier, and T.S. Bjorheim, Confinement effects for oxygen vacancies in BaZrO3 ultrathin films, Abstract: D.13.7.

A-469.E.A. Kotomin, "Ab initio calculations of defects in perovskite crystals for fuel cell applications". School-conference on "Atomistic Simulations of Functional Materials" (Moscow, Russia, May, 2016).

A-470. D. Gryaznov, R. Merkle, Yu.A. Mastrikov, E.A. Kotomin, and J. Maier, "Mechanism of the oxygen reduction reaction at SOFC cathodes: combined experimental and ab-initio investigations". – Functional Oxide Surfaces and Interfaces (FOXSI), (Vienna, Austria, May, 2016).

A-471. V.N. Kuzovkov, E.A. Kotomin, A. Lushchik, and A.I. Popov, "Diffusion-controlled kinetics of metallic colloid formation in ionic crystals". – 6th International Colloids Conference (Berlin, Germany, June, 2016). Abstract P006.

A-472. V.N. Kuzovkov, G. Zvejnieks, E.A. Kotomin, and P. Merzlyakov, "Modelling of metal colloid superlattice formation inirradiated wide gap insulators". Ibid., Abstract: P007.

A-473. V.N. Kuzovkov, E.A. Kotomin, A. Lushchik, and A.I. Popov, "The kinetics of diffusion-controlled recombination of radiation-induced defects in ionic solids".– 12th International Conference on Diffusion in Solids and Liquids, DSL 2016 (Split, Croatia, June, 2016). Abstract: DSL122.

A-474. E.A. Kotomin, Yu. Mastrikov, and J. Maier, "Structural stability of complex perovskites for solid oxide fuel cells: first principles thermodynamic calculations". – 12th International Symposium on Systems with Fast Ionic Transport, ISSFIT-12 (Kaunas, Lithuania, July, 2016). Abstracts: p. 15.

A-475. A.I. Popov, E.A.Kotomin, and J.Maier, "Analysis of the self-trapped hole mobility and recombination in alkali halides and complex metal oxides". Ibid., Abstract p. 115.

A-476. R.A. Evarestov , Yu.F. Zhukovskii, S. Piskunov, A. Platonenko, E.A. Kotomin, and J. Maier, "Ab initio simulations of interstitial oxygen in corundum" – The 19th International Conference on Defects in Insulating Materials, ICDIM'16 (Lyon, France, July, 2016). Abstract: Mo-O-15.

A-477. D. Gryaznov, R. Merkle, E.A. Kotomin, and J. Maier, "First-principles calculations of protonic defects in (La,Sr)FeO3 perovskites." - 18th International Conference on Solid State Protonic Conductors (SSPC-18), (Oslo, Norway, September, 2016). Abstracts: p.166.

A-478. E.A. Kotomin, "Ab initio calculations for oxide functional materials".— International school on Electrochemical Energy Conversion and Storage (Stuttgart, Germany, October, 2016).

A-479. A.I. Popov, Y.F. Zhukovskii, E.A. Kotomin, A. Platonenko, S. Piskunov, V.N. Kuzovkov, A. Lushchik, and R. Vila, "Computer simulations of radiation damage and defect

recombination kinetics in sapphire". — 17th Nuclear Materials Conference, (Montpellier, France, November, 2016). Abstract P.1.72.

A-480. E.A. Kotomin, V.N. Kuzovkov, and A.I. Popov, "Comparative analysis of the diffusion-controlled thermal annealing of radiation defects in simple oxides and piezoelectric PLZT ceramics". – International conference on materials science (Aveiro, Portugal, April, 2017). Abstract: p. 170.

A-481. E.A. Kotomin, M. Arrigoni, T.S. Bjorheim, and J. Maier, First principles calculations of defects in thin perovskite films.— Functional Materials and Nanotechnologies FMNT2017 (Tartu, Estonia, April 2017). Abstract: OR 6.

A-482. D. Gryaznov, R. Merkle, E.A. Kotomin, and J. Maier, First principles calculations of perovskite materials for energy applications. Ibid., Abstract: OR-29.

A-483. G. Zvejnieks, A. Anspoks, E.A. Kotomin, and V.N. Kuzovkov, Kinetic Monte-Carlo simulations of oxide nanocluster formation and growth in ODS steels. Ibid., Abstract: P-1.

A-484. A. Platonenko, D. Gryaznov, R.A. Evarestov, Yu.F. Zhukovskii, and E.A. Kotomin, Ab initio simulations on properties of O intersitials in Al2O3. Ibid., Abstract: P-19.

A-485. L. Rusevich, G. Zvejnieks, and E.A. Kotomin, First principles calculations of complex perovskite piezoelectrics. Ibid., Abstract: P-48.

A-486. A. Chesnokovs, D. Gryaznov, R.A. Evarestov, and E.A. Kotomin, First principles calculations of defective CeO2: use of site symmetry in a supercell model. Ibid., Abstract: P-76.

A-487. E.A. Kotomin, A.I. Popov, V.N. Kuzovkov, A. Moskina, A. Lushchik, E. Shablonin, and E. Vasilchenko, Theoretical analysis of the F center thermal annealing in neutron- and heavy ion irradiated Al2O3. Ibid., Abstract: P-88.

A-488. A. Gopejenko, Yu.A. Mastrikov, Yu.F. Zhukovskii, E.A. Kotomin, P.V. Vladimirov, V.A. Borodin, and A. Moeslang, Ab initio modelling of pairwise interactions of Ti solute with Y and O impurities and VFe vacancies in alfa and gamma- Fe lattices. Abstract: P-109.

A-489. E.A. Kotomin, M. Kuklja, Yu. Mastrikov, R. Merkle, J. Maier, "Large scale first principles modeling of non-stoichiometric complex perovskites for fuel cell applications"'. – 14th Symposium on Fuel Cell and Battery Modeling and Validation (ModVal-14, Karlsruhe, Germany, March 2-3, 2017). Abstr., p.42

A-490. D. Gryaznov, R. Merkle, E. A. Kotomin, J. Maier, "First principles calculations of perovskite cathode materials for protonic ceramic fuel cells", Ibid. p.32.

A-491. E.A. Kotomin, A.I. Popov, Yu.F. Zhukovskii, A. Platonenko, S. Piskunov, V.N. Kuzovkov, A.Ch. Lushchik, and R. Vila, Atomistic simulations of radiation damage and defect recombination kinetics in neutron irradiated sapphire. – 16th International Conference on Plasma-facing Materials and Components, (Dusseldorf, Germany, May 2017). Abstract: P1-61.

A-492. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M.M. Kuklja, and J. Maier, The effect of cathode surface termination on oxygen reduction reaction rate. — 231st Electrochemical Society Meeting (New Orleans, USA, May 2017), Abstract: p. 145.

A-493. D. Gryaznov, R. Merkle, E.A. Kotomin, and J. Maier, First principles calculations of perovskite cathode materials for protonic ceramic fuel cells. — 21st International Conference on Solid State Ionics (Padua, Italy, June 2017). Abstract: I-8-8-P.

A-494. T.S. Bjorheim, E.A. Kotomin, and J.Maier,Defect segregation and space-charge effects at oxide surfaces. Ibid., Abstract: IV-3-18-I.

A-495. E. A. Kotomin, M. Arrigoni, T.S. Bjorheim, and J. Maier, First principles thermodynamics of oxygen vacancies in ultrathin perovskite films. Ibid., Abstract: IV-4-1-P.

A-496. E. A. Kotomin, M. Arrigoni, T.S. Bjorheim, D. Gryaznov and J. Maier, First principles calculations of oxygen vacancies in the bulk and on surface of perovskites: a key role of phonon contribution in defect thermodynamics. Ibid., Abstract: IV-4-9-I.

A-497. V.N. Kuzovkov, E.A. Kotomin, and A.I. Popov,Kinetics of dimer F2-type center annealing in ionic solid. — 19th International Conference on Radiation Effects in Insulators, REI 19 (Versailles, France, July 2017). Abstract: p. 68.

A-498. A.I. Popov, V.N. Kuzovkov, A. Ch. Lushchik, and E.A. Kotomin, Thermal annealing of F-type color centers in irradiated oxides: A critical analysis of experimental and theoretical results. Abstract: p. 89.

A-499. E.A. Kotomin, V.N. Kuzovkov, A.I. Popov, J. Maier, and R. Vila, Anomalous kinetics of diffusion-controlled F center annealing in neutron irradiated sapphire. Abstract: p. 153.

A-500. Yu.A. Mastrikov, P.V. Vladimirov, V.A. Borodin, S. Koch, A.Gopejenko, Yu.F. Zhukovskii, E.A. Kotomin, and A.Moslang, Ab initio modeling of the Y, O solute interaction in iron matrix. Ibid., Abstract: p. 218.

A-501. A.Platonenko, D. Gryaznov, Yu.F. Zhukovskii, S. Piskunov, and E.A. Kotomin, Ab initio simulations of interstitial oxygen migration in corundum crystals. Ibid., Abstract: p. 219.

A-502. A.I. Popov, T. Kärner, N. Mironova-Ulmane, A.Ch. Lushchik, V.N. Kuzovkov, and E.A. Kotomin, Comparative analysis and theoretical modeling of the annealing of EPR and optical absorption in neutron-irradiated MgO single crystal. Ibid., Abstract: p. 240.

A-503. V.N. Kuzovkov, E.A. Kotomin, and A.I. Popov, Kinetics of dimer F2-type center annealing in ionic solids. – XX. E-MRS 2016 Fall Meeting (Warsaw, Poland, September 2017). Abstracts: E, p. 119-2.

A-504. Yu.A. Mastrikov, P.V. Vladimirov, V.A. Borodin, S. Koch, A. Gopejenko, Yu.F. Zhukovskii, E.A. Kotomin, and A. Mslang, Ab initio modelling of the Y,O solute interaction in iron matrix. Ibid., Abstracts: E, p. 119-3.

A-505. E.A. Kotomin, A.I. Popov, V.N. Kuzovkov, E. Shablonin, and A.Ch. Lushchik, Theoretical analysis of the F center thermal annealing in heavy-ion irradiated Al2O3. Ibid., Abstracts: E, p. 120-1.

A-506. A. Platonenko, D. Gryaznov, Yu.F. Zhukovskii, and E.A. Kotomin, Ab initio simulations on properties and mobility of interstitial oxygen in corundum. Ibid., Abstracts: E, p. 120-3.

A-507. G. Zvejnieks, A. Anspoks, E.A. Kotomin, and V.N. Kuzovkov. Kinetic Monte Carlo modeling of Y2O3 nanoparticle formation in radiation resistant matrices. Ibid., Abstracts: E, p. 120-5.

A-508. E.A. Kotomin, V.N. Kuzovkov, A.I. Popov, J. Maier, and R. Vila, Kinetics of diffusion-controlled F-center annealing in binary oxide materials. Ibid., Abstracts: E, p. 122-1.

A-509. E. Kotomin. "Effect of surface termination on the oxygen reduction rate on cathodes for oxide fuel cells". – The 18th Israel Materials Engineering Conference IMEC-18 (Dead Sea, Israel, February 2018). Abstracts: p. 30.

A-510 . M.F. Hoedl, R. Merkle, E. Makagon, I. Lubomirsky, E.A. Kotomin, and J. Maier. "Ab initio study of electromechanical properties of Yttrium doped Barium Zirconate". Ibid. p. 27.

A-511. G. Zvejnieks, L.L. Rusevich, D. Gryaznov, and E.A. Kotomin. "First Principles Study of (Ba,Sr)TiO3 Perovskite Solid Solutions and Heterostructures for Energy Harvesting". – EMRS 2018 Spring Meeting (Strasbourg, France, June 2018). Abstract: B.P1.31.

A-512. L.L. Rusevich, G. Zvejnieks, E.A. Kotomin, M.M. Krzmanc, S. Kunej, and I.D. Vlaicu. "Theoretical and experimental study of BaTiO3-based composite perovskites for energy harvesting applications". Ibid., Abstract: B.P1.32.

A-513. A. Platonenko, Yu.F. Zhukovskii, D. Gryaznov, and E.A. Kotomin. "Ab initio study of oxygen interstitials in MgAl2O4 spinel". Ibid., Abstract: K.4K.6.

A-514. A.I. Popov, V.N. Kuzovkov, A.Ch. Lushchik, and E.A. Kotomin. "Thermal annealing of F-type centers in irradiated oxides: A critical analysis of experimental and theoretical studies". Ibid., Abstract: K.V.3.

A-515. Yu.A. Mastrikov, M.N. Sokolov, E.A. Kotomin, A.V. Gopejenko, and Yu.F. Zhukovskii. "Ab initio modelling of Y and O solute atom interaction in small clusters within the bcc iron lattice". Abstract: K.PI.5.

A-516. A.I. Popov, M. Izerrouken, V.N. Kuzovkov, A.Ch. Lushchik, E.A. Kotomin, and R. Vila. "Modeling of F-type centers thermal annealing in irradiated Al2O3". Ibid., Abstract: K.PI.6.

A-517. A. Chesnokov, D. Gryaznov, and E.A. Kotomin. "First principles calculations of CeO2 doped with Tb".Ibid., Abstract: K.XV.3.

A-518. E.A. Kotomin, Yu.A. Mastrikov, R. Merkle, M.M. Kuklja, and J. Maier. "Effect of the cathode surface termination on the oxygen reduction reaction rate". Ibid., Abstract: R.9.5.

A-519. D. Gryaznov, M. Hodl, R. Merkle, E.A. Kotomin, and J. Maier. "First principles calculations of protonic defects in ferrate perovskites". Ibid., Abstract: R.P2.3.

A-520. Ju. Garcia-Fayos, D. Gryaznov, D. Catalan, E.A. Kotomin, and J.M. Serra. "CO2 adsorption on perovskite membranes and its effect on oxygen permeation". Ibid., Abstract: R.P2.4.

A-521. A.I. Popov, E.A. Kotomin, D. Gryaznov, and J. Maier. "Are color centers possible in ceria?". Ibid., Abstract: R.P2.8.

A-522. M.F. Hoedl, R. Merkle, E. Makagon, I. Lubomirsky, E.A. Kotomin, J. Maier. "Acceptor-doped BaZrO3: Ab-initio study of (electro)mechanical properties". Ibid., Abstract: R.11.5.

A-523. E.A. Kotomin, V.N. Kuzovkov, and A.I. Popov. "Unusual kinetics of F center annealing in irradiated oxide materials". Ibid., Abstract: Y.1.2.

A-524. A.I. Popov, E.A. Kotomin, V.N. Kuzovkov, and A. Lushchik. "Thermal annealing of F type centers in irradiated solids".— The Europhysical Conference on Defects in Insulating Materials (Eurodim) (Bydgoszcz, Poland, 8-13 July). Abstracts, p. 10.

A-525. E.A. Kotomin, M. Kuklja, Yu.A. Mastrikov, R. Merkle, and J.Maier. Large scale first principles modelling of non-stoichiometric perovsites. Ibid., Abstracts, p. 13.

A-526. D. Gryaznov, M.F. Hdl, R. Merkle, E.A. Kotomin, and J. Maier. Proton uptake and mobility in (Ba,Sr,La)FeO3 perovskites: DFT results. Ibid., Abstracts, Nr. TuP1-10, p.16.

A-527. M. Hoedl, R. Merkle, E. Makagon, I. Lubomirsky, E.A. Kotomin, and J.Maier. DFT investigation of (electro)mechanical properties of Y- and Sc-doped BaZrO3. — Electroceramics XVI (Hasselt, Belgium, 9-12 July). Abstract PS-1C.05, p. 17.

A-528. E. Makagon, M. Hoedl, R. Merkle, E.A. Kotomin, J.Maier, and I. Lubomirsky. Mechanical and electromechanical properties of acceptor doped BaZrO3. Ibid., Abstract OS-4B.03, p.22.

A-529. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, and J. Maier. "Effects of the surface termination on oxygen reduction rate on cathodes for fuel cells". — International conference on atomistic simulations of functional materials ASFM-2018 (Moscow, Russia, 12-13 September).Abstracts.

A-530. A.I. Popov, E.A. Kotomin, V.N. Kuzovkov, and A. Lushchik. "Radiation effects and defect annealing in functional materials for fusion applications". — 6th International Congress on Energy Fluxes and Radiation Effects EFRE-2018 (Tomsk, Russia, 16-22 September 2018). Abstracts: p.13.

A-531. A.B. Usseinov, Yu.F. Zhukovskii, E.A. Kotomin, A.T. Akilbekov, M.V. Zdorovets, and G.M. Baubekova. "Transition levels of acceptor impurities in ZnO crystal by DFT-LCAO calculations". Ibid., Abstracts: p.652.

A-532. A.I. Popov, E.A. Kotomin, and V.N. Kuzovkov. "Understanding of the kinetics of defect annealing in heavily irradiated binary and complex oxides disordering effects". — 12th International Conference of Functional Materials and Nanotechnologies FMNT-2018 (Riga, Latvia, 2-5 October 2018). Abstract OR-4.

A-533. A. Sternberg, A.I. Popov, E.A. Kotomin, A. Anspoks, and J. Purans. "Advanced materials and technologies in fusion research: an overview and some recent results from Latvian EUROfusion laboratory". Ibid., Abstract OR-26, p.99.

A-534 . E.A. Kotomin, M. Kuklja, Yu. Mastrikov, R. Merkle, and J. Maier. "First principles calculations of perovskite solid solutions for fuel cells". Ibid., Abstract OR-28, p.101.

A-535. D. Gryaznov and E.A. Kotomin. "CO2 adsorption on mixed ionic-electronic conducting membranes". Ibid., Abstract PO-6, p.116.

A-536. A.I. Popov, E.A. Kotomin, A.Moskina, and V.N. Kuzovkov. "Modeling of F-type centers thermal annealing in neutron irradiated and thermochemically reduced BeO". Ibid., Abstract PO-11, p.121.

A-537. L.L. Rusevich, G. Zvejnieks, and E.A. Kotomin. "Ab initio simulation of (Ba,Sr/Ca)TiO3 composite perovskites". Ibid., Abstract PO-15, p.125.

A-538. D. Zablotsky, V.N. Kuzovkov, and E.A. Kotomin. "Dipole-induced disorder in quasi-equilibrium assemblies of ferroelectric nanocubes". Ibid., Abstract PO-18, p.128.

A-539. L.L. Rusevich, G. Zvejnieks, E.A. Kotomin, M.M. Krzmanc, S. Kunej, and I. Vlaicu. "Theoretical and experimental study of BaTiO3-based perovskites solid solutions and BaTiO3/SrTiO3 heterostructures". —10th International Conference and Exposition on Electrical and Power Engineering EPE-2018 (Iasi, Romania, 18-19 October 2018). Program, p.9.

A-540. T.S. Bjorheim, M. Hoedl, E.A. Kotomin, R. Merkle, J. Maier. "Defect thermodynamics and lattice site basicity in mixed conducting oxides". — International Conference "Non-Stoichiometric Compounds VII" (Phoenix Seagaia Resort, Miyazaki (Kyushu Island), Japan, 10-14 March 2019).Abstract: p.28.

A-541. M. Hoedl, R. Merkle, E.A. Kotomin, J. Maier. "Proton uptake in the mixed ionic and electronic conductors Ba1-xSrxFeO3". Ibid.,

A-542. D. Gryaznov, M.F. Hoedl, R. Merkle, E.A. Kotomin, J. Maier. "DFT+U calculations of protonic defects in (Ba,Sr)FeO3-delta". – 16th Symposium on Modeling and Experimental Validation of Electrochemical Energy Technologies ModVal-2019 (Braunschweig, Germany, 12-13 March 2019). Abstract: p.50.

A-543. A.I. Popov, E.A. Kotomin, V.N. Kuzovkov. "Thermal annealing of radiation damage in binary and complex oxides". — International Workshop on Advanced Magnetic Oxides IWAMO-2019 (Aveiro, Portugal, 15-17 April 2019). Workshop Book: p.62.

A-544. A.I. Popov, E.A. Kotomin, V.N. Kuzovkov. "Understanding of the kinetics of defect annealing in heavily irradiated binary and complex oxides disordering effects". — E-MRS 2019 Spring Meeting (Nice, France, 27-31 May 2019). Abstract J P1.5.

A-545. A.I. Popov, E.A. Kotomin, V.N. Kuzovkov. "Modeling of F-type centers thermal annealing in neutron irradiated and thermochemically reduced ZnO and BeO single crystals". Ibid., Abstract J P1.9.

A-546. V.N. Kuzovkov, A.I. Popov, E.A. Kotomin, M. Izerrouken, R. Villa. "Comparison of the F-type center thermal annealing in irradiated Al2O3 and Y3Al5O12 single crystals". Ibid., Abstract J P1.30.

A-547. S. Piskunov, I. Isakovica, A.I. Popov, E.A. Kotomin. "Phase transition at stepped SrTiO3 low index surfaces: Prediction from the first principles".Ibid., Abstract AA P.34.

A-548. D. Zablotsky, V.N. Kuzovkov, E.A. Kotomin. "Manifestation of intrinsic dipoles in the evaporation-driven assembly of perovskite nanocubes into energy harvesting composites". Ibid., Abstract P 2.24.

A-549. M.F. Hoedl, D. Gryaznov, R. Merkle, E.A. Kotomin, J. Maier. "Acid-base properties of triple conducting Ba1-xSrxFeO3-delta perovskites". — 118th General Assembly of the German Bunsen Society for Physical Chemistry BUNSENTAGUNG-2019 (Jena, Germany, 30 May 1 June 2019). Abstract P01.36, p.308.

A-550. G. Zvejnieks, D. Zavickis, D. Gryaznov, E.A. Kotomin. "The electronic structure of LaCoO3 and BaCoO3 perovskites". – Ibid., Abstract P08.03, p.494.

A-551. A. Chesnokov, D. Gryaznov, E.A. Kotomin. "Calculating Tb3+-doped CeO2 from first principles". Ibid., Abstract P08.09, p.500.

A-552. G. Zvejnieks, L.L. Rusevich, D. Gryaznov, E.A. Kotomin. "First principles study of structural and piezoelectric properties of SrTiO3/BaTiO3 heterostructures". Ibid., Abstract P08.14, p.505.

A-553. M.F. Hoedl, D. Gryaznov, R. Merkle, E.A. Kotomin, J. Maier. "DFT investigations of triple conducting (Ba,Sr)FeO3-delta cathode materials". —- 22nd International Conference on Solid State Ionics (PyeongChang Alpensia Resort, Korea, 16-21 June 2019). Abstract: p.48.

A-554. R. Merkle, R. Zohourian, G. Raimondi, M.F. Hoedl, E.A. Kotomin, F. Giannici, A. Chiara, A. Longo, A. Martorana, J. Maier. "Proton uptake in mixed conducting perovskites". Ibid., Abstract SO-075, p.49.

A-555. V.N. Kuzovkov, A.I. Popov, E.A. Kotomin. "Anomalous diffusion in irradiated oxide crystals ". —- 15th International Conference on Diffusion in Solids and Liquids - DSL2019 (Athens, Greece, 24-28 June 2019). Abstract P-97.

A-556. R.Merkle, R.Zohourian, G.Raimondi, M.Hoedl, E.A.Kotomin, J.Maier. "Mixed conducting PCFC cathode materials: proton uptake, proton mobility, and defect interactions". —- IEEE International Symposium on Applications of Ferroelectrics - ISAF (EPFL Lausanne, Switzerland, 14-19 July 2019). Abstract ThORiii2BC.1, p.90.

A-557. M.Hoedl, E.Makagon, I. Lubomirsky, R.Merkle, E.A.Kotomin, J.Maier. "Influence of dopants and hydration on the elastic properties of BaZrO3". Ibid., Abstract ThPOiiPosters.33, p.95.

A-558. G. Baubekova, A. Akilbekov, E.A. Kotomin, V.N. Kuzovkov, A. Lushchik, A.I. Popov, M. Zdorovets, E. Vasilchenko. "Thermal annealing of radiation damage caused by swift 132Xe ions in MgO single crystals". — 20th International Conference on Radiation Effects in Insulators REI-20 (Nur Sultan (Astana), Kazakhstan, 1923 August 2019). Abstract P.1.30, Book of Abstracts, p.112.

A-559. E.A. Kotomin, V.N. Kuzovkov, A.I. Popov, M. Izerrouken, R. Villa. "Peculiarities of defect recombination kinetics in irradiated Al2O3 and Y3Al5O12 single crystals". Ibid., Abstract P.1.33, Book of Abstracts, p.115.

A-560. E.A. Kotomin, A.I. Popov, D. Gryaznov, J. Maier. "Could color centers exist in CeO2". Ibid., Abstract P.1.34, Book of Abstracts, p.116.

A-561. A. Platonenko, D. Gryaznov, E.A. Kotomin, A. Lushchik, A.I. Popov, V. Seeman. "Experimental and theoretical study of the structural, electronic and vibrational properties of radiation defects in magnesium aluminate spinel". ibid. Abstract P.1.36, Book of Abstracts, p.118.

A-561. A. Lushchik, E.A. Kotomin, V.N. Kuzovkov, A.I. Popov, G. Prieditis, V. Seeman, E. Shablonin. "Annealing kinetics of the F-centers in irradiated MgAl2O4 spinel". Ibid., Abstract P.1.37, Book of Abstracts, p.119.

A-562. E. Elsts, V.Kuzovkov, E. Kotomin, S. Pazylbek, A.I. Popov. "Thermal annealing of defects in MgF2 single crystals induced by neutrons at low temperatures". Ibid., Abstract P.1.40, Book of Abstracts, p.122.

A-563. A.I. Popov, A. Lushchik, R. Vila, E.A. Kotomin. "Radiation defects and processes in ionic oxides where we are standing now and what we understand better". Ibid., Abstract P.1.54, Book of Abstracts, p.136.

A-564. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M.M. Kuklja, J. Maier. "Role of surface termination and defects on oxygen reduction reaction rate in solid oxide fuel cells". Ibid., Abstract P.2.52, Book of Abstracts, p.204.

A-565. A. Sternberg, A.I. Popov, E.A. Kotomin. "Advanced materials and technologies in fusion research: An overview and some recent results from Latvian EUROfusion laboratory". Ibid., Abstract P.2.55, Book of Abstracts, p.207.

A-566. A.I. Popov, E.A. Kotomin, A. Moskina, V.N. Kuzovkov. "Modeling of F-type centers thermal annealing in neutron irradiated and thermochemically reduced BeO". Ibid., Abstract P.2.62, Book of Abstracts, p.214.

A-567. Popov A.I., Kotomin E.A., Kuzovkov V.N. "Point defect aggregation and metallic nanocolloid formation in ionic solids". — 7th International Conference "Nanotechnologies and Nanomaterials" NANO-2019 (Kiev, Ukraine, 27 -30 August 2019). Book of Abstract: p.702. A-568. Kotomin E.A, Merkle R., Mastrikov Yu., Maier J. Prediction of oxygen reduction reaction kinetics at fuel cell cathodes: First principles calculations. — Americal Ceramic Society Meeting (Orlando, January 2020), Abstracts of Symposium S14 Agile design of Electronic Materials).

A-569. E.A. Kotomin. Computer modelling of radiation-induced processes in oxide solids- — 7th International Congress on Energy Fluxes and Radiation Effects EFRE-2020 (Tomsk, Russia, 14-26 September 2020).

A-570. A. Chesnokov, D. Gryaznov, J. Purans, E.A. Kotomin, N.V. Skorodumova. Role of interstitial oxygens in Ir-doped ZnO — International Online Conference of Functional Materials and Nanotechnologies FMNT-2020 (Vilnius, Lithuania, 23-26 November, 2020), Abstract book, p.35.

A-571. Yu.A. Mastrikov, E.A. Kotomin. "Modelling of oxygen reduction reaction at solid oxide fuel cell cathode". Ibid., Abstract S4-2, Abstract book, p.48.

A-572. A.I. Popov, E.A. Kotomin. "Radiation-induced point defects and processes in ionic oxides where we are standing now and what we understand better". Ibid., Abstract book, p.57.

A-573. N. Krainyukova, V. Hamalii, . Popov, E. Kotomin. "In-plane lattice parameters and structural transitions on SrTiO3 (001) surface at low temperatures". Ibid., Abstract book, p.123.

A-574. Yu.A. Mastrikov, G. Zvejnieks, L.L. Rusevich, E.A. Kotomin. "First principles modelling of water adsorption and dissociation on flat and faceted SrTiO3 surfaces". Ibid., Abstract book, p.126.

A-575. L.L. Rusevich, G. Zvejnieks, Yu.A. Mastrikov, E.. Kotomin, M. Macek Krzmanc. "Band gap engineering of SrTiO3 photocatalyst for sunlight-driven water splitting: ab initio simulations". Ibid., Abstract book, p.127.

A-576. A. I. Popov, I. Makarenko, Yu. Mastrikov, E.A. Kotomin. "Case analysis of self-trapped hole Vk center mobility in metal fluorides and fluoroperovskites". Ibid., Abstract book, p.166.

A-577. D. Zavickis, G. Zvejnieks, E. Kotomin, D. Gryaznov. "Characterization of Co ion oxidation state and local structural distortions in BaCoO3". Ibid., Abstract book, p.175.

A-578. Makagon, M. Hoedl, R. Merkle, E.A. Kotomin, J. Maier, I. Lubomirsky. "Non-classical electrostrictive phenomena in hydrated acceptor doped BaZrO3: Proton trapping and dopant size effect". — IEEE International Symposium on Applications of Ferroelectrics ISAF (Sidney, Australia, 16-21 May 2021). Abstract 3003. OR.

A-579. D. Gryaznov, R. Merkle, M.F. Hoedl, E.A. Kotomin, J. Maier. "First-principles calculations of protonic defects in (Ba,Sr,La)(Fe,Co)O3-delta perovskite oxides". — E-MRS 2021 Spring Meeting (Virtual Conference, 31 May - 4 June 2021). Abstract G.We1.3.

A-580. R. Merkle, M.F. Hoedl, G. Raimondi, E.A. Kotomin, J. Maier. "Mixed conducting PCFC cathode materials with protons, oxygen vacancies and holes: Detailed defect-chemical understanding". Ibid, Abstract G.We2.1.

A-581. E.A. Kotomin, R.A. Evarestov, J. Maier. "First-principles calculations of defects in CsPbX3 (X = Br, I) crystals". Ibid, Abstract J.I.1.

A-582. A. Chesnokov, D. Gryaznov, E.A. Kotomin, J. Purans. "Thermoelectric properties of Ir-doped ZnO from hybrid DFT calculations". Ibid., Abstract J.IV.2.

A-583. A. Platonenko, D. Gryaznov, A.I. Popov, E.A. Kotomin. "Ab initio study of the vibrational properties of F-type centers in oxide and halide crystals: case study of Al2O3 and KBr". Ibid., Abstract J.IV.7.

A-584. E. Makagon, M.F. Hoedl, R. Merkle, E.A. Kotomin, J. Maier, I. Lubomirsky. "Non-classical electrostrictive phenomena in hydrated acceptor doped BaZrO3: Proton trapping and dopant size effect". Ibid., Abstract J.IX.3.

A-585. D. Gryaznov, E.A. Kotomin, A. Platonenko, A. Popov. "First principles calculations of defect formation energies and oxide crystals". Ibid, Abstract J.IX.9.

A-586. Yu.A. Mastrikov, N.G. Chuklina, A.I. Popov, E.A. Kotomin, D.V. Gryaznov. "Small polarons in PbX2 (X= F, Cl, Br): computational study". Ibid., Abstract J.XI.5.

A-589. A. Platonenko, D. Gryaznov, A. Lushchik, A. I. Popov, E. K. Kotomin. "A comprehensive hybrid DFT study on oxygen interstitial behavior in Al2O3". Ibid, Abstract L.3.2.

A-580. G. Zvejnieks, D. Zavickis, E. A. Kotomin, D. Gryaznov. "Monoclinic ground state of BaCoO3: first principles studies". Ibid, Abstract G.Mo.12.

A-591. T.S. Bjorheim, M.F. Hoedl, R. Merkle, E.A. Kotomin, J. Maier. "Proton, hydroxide ion, and oxide ion affinities of closed-shell oxides and its relation to electronic structure". Ibid., Abstract G.We.Poster.4

A-592. L.L. Rusevich, G. Zvejnieks, E.. Kotomin, M. Macek Krzmanc. Defect-induced variation of SrTiO3 band gap for photocatalytic applications: first-principles simulations. Ibid., Abstract J.PI.13.

A-593. L.L. Rusevich, G. Zvejnieks, E.A. Kotomin, A.I. Popov, T. Scherer. "First principles calculations of the atomic, electronic and vibrational properties of defective diamond". Ibid., Abstract J.PI.15.

A-594. A. Lushchik, V.N. Kuzovkov, A.I. Popov, G. Prieditis, V. Seeman, E. Shablonin, E. Vasilchenko, E.A. Kotomin. "Evidence for the radiation-induced formation of two types of oxygen interstitials in sapphire single crystals". Ibid., Abstract J.PII.8.

A-595. N.V. Krainyukova, V.O. Hamalii, A.I. Popov, L.L. Rusevich, E.A. Kotomin. "In-plane contraction and structural transformations on the SrTiO3 (001) surface". Ibid., Abstract J.PII.9. .

A-596. G. Zvejnieks, L.L. Rusevich, E.A. Kotomin, M. Macek Krzmanc. "Challenges of interpretation of Bi4Ti3O12 within orthorhombic space groups". Ibid. Abstract J.PII.12.

A-597. L.L. Rusevich, D. Gryaznov, E.. Kotomin, V. Krasnenko. Defect-induced properties of thin perovskite films: first-principles simulations. Ibid, Abstract J.PII.16.

A-598. A.I. Popov, V.N. Kuzovkov, A. Platonenko, E. Elsts, A.Moskina, E.A. Kotomin. "Comparative analysis of radiation defect annealing in scintillator materials for high-energy physics and medical applications".Ibid, Abstract J.PII.31.

A-599. M.F. Hoedl, R. Merkle, E. Kotomin, J. Maier. "Proton uptake and defect interactions in mixed conducting BaxSr1-xFeO3". —- Solid State Proton Conductors (SSPC-20) Online Conference (27.9. - 1.10.2021). Abstract 9-O, Book of Abstracts, p.13.

A-600. E. Makagon, M. Hoedl, R. Merkle, E. Kotomin, J. Maier, I. Lubomirsky. "Non-classical electrostrictive phenomena in hydrated acceptor doped BaZrO3: proton trapping and dopant size effect". Ibid., Abstract 60-O, p.123.

A-601. E.A. Kotomin, V.N. Kuzovkov, A.I. Popov, D. Gryaznov, A. Platonenko, R. Vila. "Modelling of radiation-induced processes in advanced oxide solids".— International Conference on Fusion Reactor Materials ICFRM-20 (Online Conference, 24-29 October 2021). Abstract No.392.

A-602. E.A. Kotomin, A.I. Popov, V.N. Kuzovkov, A. Platonenko. "First principles calculations of the electronic and magnetic properties for defects in oxide crystals".—

2nd International Workshop on Advanced Magnetic Oxides IWAMO-2021 (Online, 24-26 November 2021).

A-603. A. Lushchik, V. Seeman, E. Shablonin, E. Vasil'chenko, E.A. Kotomin, V.N. Kuzovkov, A.I. Popov. "Detection of uncatchable oxygen interstitials in neutron-irradiated corundum crystals". 11th International Conference on Luminescent Detectors and Transformers of Ionizing Radiation LUMDETR-2021 (Bydgoszcz, Poland, 12-17 September 2021).– Abstract WeS8-K17, p.62. INV.R.

A-604. A.I. Popov, E.A. Kotomin. "Striking lattice parameter-dependent features in the delocalization of self-trapped hole centers Vk in binary and complex halides". XVIII YOUTH CONFERENCE WITH INTERNATIONAL PARTICIPATION ON LUMINESCENCE AND LASER PHYSICS (LLPH-2021) (5 10 July 2021, Irkutsk, Russia).INV.R.

A-605. A.I. Popov, E.A. Kotomin, V.N. Kuzovkov, A. Lushchik. "Thermal Annealing of Point Defects in Irradiated Functional Ceramics for Nuclear Applications". 6TH INTERNATIONAL CONFERENCE ON OXIDE MATERIALS FOR ELECTRONIC ENGINEERING FABRICATION, PROPERTIES AND APPLICATION (28 September - 2 October 2021, Lviv, Ukraine).INV.R.

A-606. Yu.A. Mastrikov, M.N. Sokolov, V.P. Krasnenko, E.A. Kotomin. "Water adsorption on strontium titanate stepped surface". INV.R. Annual meeting of the COST Action: Computational materials sciences for efficient water splitting with nanocrystals from abundant elements (CA18234) Computational water splitting, where we are now and where to go?" (Online event, 14-15 February 2022).

A-607. M. Hoedl, R. Merkle, E. Kotomin, J. Maier. "Defect chemistry of BaFeO3 cathode materials investigated by density functional theory". — 6th International workshop on Prospects on protonic ceramic cells PPCC-2022 (Dijon, France, 8-10 June 2022).

A-608. V.N. Kuzovkov, A.I. Popov, E.A. Kotomin. "Understanding diffusion-controlled recombination kinetics in heavily irradiated binary and complex oxides". Abstract book, p.54. PR. — 18th International Conference on Diffusion in Solids and Liquids - DSL2022 (Florence, Italy, 27 June - 1 July 2022).

A-609 .M.F. Hoedl, A. Chesnokov, R. Merkle, D. Gryaznov, E.A. Kotomin, J. Maier. "First-principles study of proton diffusion in BaFeO3". INV-21, Book of abstracts, p. 82. — Joint International Conference FMNT-NIBS 2022 (Riga, Latvia, 3-6 July 2022).

A-610. E.A. Kotomin, A.I. Popov, V.N. Kuzovkov, A. Platonenko. "First principles calculations of radiation defect properties in complex oxide crystals".Ibid., INV-22, Book of abstracts, p. 83. INV.R.

A-611. A.I. Popov, E.A. Kotomin, V.N. Kuzovkov, A. Lushchik, A. Platonenko, E. Shablonin, V. Seeman, T.A. Scherer. "Deep understanding of advanced optical and dielectric materials for fusion diagnostic applications". Ibid., INV-26, Book of abstracts, p. 87. INV.R.

A-612. D. Gryaznov, M. Hoedl, R. Merkle, E.A. Kotomin, J. Maier. "Ab-initio modelling elucidates materials trends for electrochemistri applications". Ibid., OR-34, Book of abstracts, p. 124. OR.

A-613. L.L. Rusevich, E.A. Kotomin, G. Zvejnieks, Yu.A. Mastrikov, M. Sokolov, J. Maier. "COMPUTER MODELLING OF WATER SPLITTING ON PEROVSKITE NANOPARTICLES". Ibid., Po-11, Book of abstracts, p. 145. PR.

A-614. M.F. Hoedl, R. Merkle, E.A. Kotomin, J. Maier. "THE ORBITAL NATURE OF ELECTRON HOLES IN BAFEO3 AND IMPLICATIONS FOR DEFECT CHEMISTRY". Ibid., Po-45, Book of abstracts, p. 179. PR.

A-615. R. Merkle, G. Raimondi, M. Hoedl, A. Chesnokov, D. Gryaznov, E. Kotomin, J. Maier. "Mixed Proton/Hole/Oxygen Vacancy Conductors Bulk Defect Chemistry, Transport Properties and Surface Reaction Aspects". — 23rd International Conference on Solid State Ionics (Boston, USA, 17-22 July 2022). Abstract EI08.01. INV.R.

A-616. P. Rosander, M. Hoedl, R. Merkle, G. Wahnstroem, E. Kotomin, J. Miaer. "Hydration Entropy of Triple Conducting Perovskites Correlations Derived from DFT Calculations and Experimental Data". – Ibid., Abstract DT18.06. PR

A-617. A.I. Popov, E.A. Kotomin, V.N. Kuzovkov, A. Lushchik, T.A. Scherer. "Deep understanding of advanced optical and dielectric materials for fusion diagnostic applications".— DPG (German Physical Society) Meeting of the Condensed Matter Section (Regensburg, Germany, 4-9 September 2022). INV.R.

A-618. A.I. Popov, V. Kuzovkov, E.A. Kotomin, A. Lushchik. "Radiation-induced point defects and processes in ionic oxides – where we are standing now and what we understand better".— E-MRS 2022 Fall Meeting (Warsaw, Poland, 19-22 September 2022). M.P.42, PR.

A-619. COST action 18234 Conference "Design The Future: Electro-, Photo- and Thermochemical water splitting" (Brussels, Belgium, 20-22 February 2023). E.A. Kotomin. "The perovskite band engineering for photostimulated water splitting". OR.

A-620. E-MRS 2023 Spring Meeting (Strasbourg, France, 29 May - 2 June 2023). E.A. Kotomin, D. Moia, J. Maier. "First-principles calculations of defects in CsPbX3 (X = Br, I) crystals for photovoltaic applications". D2-13-571, Conference Program. OR

A-621. E.A. Kotomin, L.L. Rusevich, G. Zvejnieks, Yu. Mastrikov, M. Sokolov. "The perovskite band gap engineering for photostimulated water splitting". D-P03-69-570, Conference Program. PR.

A-622. L.L. Rusevich, E.A. Kotomin, M. Tyunina. "The electronic and dielectric properties of SrTiO3 perovskite crystals with oxygen vacancies and nitrogen impurities: First principles simulations". E-P-10-753, Conference Program. PR.

A-623. L.L. Rusevich, G. Zvejnieks, E.A. Kotomin, A.I. Popov, T. Scherer. "First principles calculations of the electronic, vibrational and dielectric properties of defective diamond". R-P-05-754, Conference Program. PR.

A-624. Defect chemistry workshop "Petite XII" (France, September 2023). R. Merkle, M.F. Hoedl, G. Raimondi, C. Berger, E.A. Kotomin, J. Maier. "Proton mobility in triple-conducting perovskites". OR.

A-625. The 21st International Conference Solid State Protonic Conductors SSPC-21 (Fukuoka, Japan, 17-22 September 2023). R. Merkle, M.F. Hoedl, G. Raimondi, C.

Berger, E.A. Kotomin, J. Maier. "Proton concentration and mobility in triple-conducting perovskites". INV.

A-626. 3rd ELSICS workshop and Bunsen-Colloquium "Energy Landscapes and Structure in Ion Conducting Solids" (Magburg, Germany, 4-6 October, 2023). R. Merkle, M.F. Hoedl, A. Chesnokov, D. Gryaznov, E.A. Kotomin, J. Maier. "Energy landscape and proton mobility in triple-conducting BaFeO3 perovskites". OR.

A-627. 6th workshop on High Performance Computing in Science and Engineering (Stuttgart, Germany, 12-13 October 2023). M.Sokolov, Yu.Mastrikov, E.Kotomin, J.Maier. "Large scale ab initio modelling of hydrogen production on stepped surfaces of SrTiO3 nanoparticles". OR.

A-628. 21st International Conference on Fusion Reactor Materials ICFRM21 (Granada, Spain, 22-27 October 2023). V. Kuzovkov, E. Kotomin, R. Vila. "Theoretical analysis of thermal annealing kinetics of radiation defects in silica". Book of Abstracts, p.482 (topic H - P46). PR.

A-629. 82nd International Scientific Conference of University of Latvia "USE OF HIGH PERFORMANCE COMPUTING IN NUMERICAL SIMULATIONS" (Riga, Latvia, 22 February 2024). M. Sokolov, Yu.A. Mastrikov, G. Zvejnieks, E.A. Kotomin. "Modeling of hydrogen production on stepped surfaces of SrTiO3 perovskite nanoparticles - ab initio computational study". Book of Abstracts. OR.

A-630. Flair conference (Seehem-Jrgenheim, Germany, 3 March 2024). R. Merkle, G. Raimondi, M.F. Hoedl, A. Chesnokov, D, Gryaznov, E.A. Kotomin, J. Maier. "Mixed-conducting barium ferrate perovskites: proton concentration and mobility". OR.

A-631. 6th International Workshop: prospects on protonic ceramic cells (Dijon, France, 8-10 June 2024). R. Merkle, M.F. Hoedl, A. Chesnokov, C. Berger, G. Raimondi T. Acatrk, U. Starke, D. Gryaznov, E.A. Kotomin J. Maier. "Proton mobility in triple-conducting perovskites -insights from experiment and theory". OR.

A-632. 12th INTERNATIONAL CONFERENCE on Luminescent Detectors and Transformers of Ionizing Radiation LUMDETR-2024 (Riga, Latvia, 16-21 June 2024). L.L. RUSEVICH, I. CHERVYAKOV, E.A. KOTOMIN, I. MIKHAILOV, D. BOCHAROV, M.G. BRIK. "First principles calculations of the advanced phosphor materials". PB07, Book of Abstracts, p.124. P

A-633. 24th International Conference on Solid State Ionics - SSI24 (London, UK, 15-19 July 2024). R. Merkle, M.F. Hoedl, A. Chesnokov, C. Berger, G. Raimondi, T. Acatrk, U. Starke, D. Gryaznov, E.A. Kotomin, J. Maier. "Proton mobility in triple-conducting perovskites - insights from experiment and theory". OR.

A-634. ElectroCeramics XIX Conference (Vilnius, Lithuania, 19-22 August 2024). R. Merkle, M.F. Hoedl, A. Chesnokov, C. Berger, G. Raimondi, T. Acartrk, U. Starke, D. Gryaznov, E.A. Kotomin, J. Maier. "Protons in mixed-conducting perovskites: Why, how many, and how fast?". Conference program. OR.

A-635. R. Merkle, A. Chesnokov, M.F. Hoedl, D. Gryaznov, C. Nader, A. Egger, E. Bucher, E.A. Kotomin, W. Sitte, J. Maier. "Electronic structure, phase formation, and defect distribution in the Ba(Ce,Fe,Acc)O3-d System".

A-636. Workshop "Advances in modelling defects in solids and interfaces" (London, UK, 14-15 October 2024). E.A. Kotomin, L.L. Rusevich, G. Zvejnieks, Yu.A. Mastrikov, M. Sokolov. "Doping effects in nanoperovskites for hydrogen production". INV.R.

A-637. Materals Research Society (MRS) meeting (Boston, USA, 1-6 November 2024). R. Merkle, M.F. Hoedl, G. Raimondi, C. Berger, A. Chesnokov, D. Gryaznov, E.A. Kotomin, J. Maier. "Protons in triple-conducting perovskites: concentration, mobility and surface reaction aspects". OR.

A-638. 41st International Scientific Conference of ISSP UL (Riga, Latvia, 3-7 March, 2025). Chervyakov, L.L. Rusevich, M.G. Brik, D. Gryaznov, A.M. Srivastava, G. Zvejnieks, D. Bocharov, M. Putnia, E.A. Kotomin. "Computational study of elastic and electronic properties of ASiF (A = Na, K, Cs) hexafluorosilicates under hydrostatic pressure". OR.

A-639. E-MRS 2025 Spring Meeting (Strasbourg, France, 26-30 May 2025). W. Sitte, R. Merkle, A. Chesnokov, D. Gryaznov, C. Nader, A. Egger, E. Bucher, E. Kotomin, J. Maier. "Triple-conducting Ba(Ce,Fe,Acc)O3- composites: phase formation, defect distribution and electronic structure investigated by density functional theory calculations". OR.

A-640. Ibid., L.L. Rusevich, G. Zvejnieks, E.. Kotomin. "Cationic substitutions by transition metal atoms in SrTiO3: first-principles simulations". OR.

A-641. Yu.A. Mastrikov, D. Gryaznov, A. Chesnokov, G. Zvejnieks, E.A. Kotomin. "Oxygen defects in Sr2FeO4- (:0-0.5): insights from DFT calculations". OR.

A-642. Y.-P. Liu, M.L. Weber, D. Jennings, L.L. Rusevich, E. Kotomin, F. Gunkel, R. Dittmann. "Phase-separation in the initial growth stage of exsolution-active SrTi0.95-xNi0.05NbxO3- thin films probed by low-temperature Scanning Tunneling Microscopy". PR.

A-643. L.L. Rusevich, G. Zvejnieks, E.A. Kotomin, M.G. Brik. "First principles study of advanced phosphors Cs2SiF6 and K2SiF6: Critical comparison of pure and Mn doped materials". PR.

A-644. E.A. Kotomin, G. Zvejnieks, L.L. Rusevich, N. Daneu, M.M. Krmanc. "First principle studies of SrTiO3 engineering with Bi based heterostructures for efficient photostimulated hydrogen production". PR.

A-645. D. Gryaznov, A. Chesnokov, E.A. Kotomin, R. Merkle. "Proton migration properties in doped and undoped BaFeO3: insights from DFT calculations". PR.

A-646. D. Gryaznov, A. Platonenko, V.N. Kuzovkov, E.A. Kotomin, A. Lushchik. "Oxygen interstitials in wide band gap oxides: hybrid DFT calculations and analysis". PR.

A-647. E.A. Kotomin, V.N. Kuzovkov, A. Lushchik, A. Podelinska, V. Seeman, E. Shablonin. "Open questions on the thermal stability of primary electronic centers in heavy swift ion irradiated MgO single crystals". PR.

22nd International Conference in Radiation Effects on Insulators REI-22 (Madrid, Spain, 8-13 June 2025).

A-648. E.A. Kotomin, V.N. Kuzovkov, A.I. Popov, D. Gryaznov, A. Platonenko, R. Vila. "Multiscale computer modelling of radiation-induced processes in advanced oxide solids". Book of Abstracts, IO02016. OR.

A-649. Z.T. Karipbayev, K. Kumarbekov, A. Akilbekov, A. Zhunusbekov, B. Aizat, A. Zhalgas, A.I. Popov. "Radiation-induced color centers in Kr ion-irradiated YAP crystals". Book of Abstracts, IP08159. PR.

21st International Conference on Diffusion in Solids and Liquids DSL-2025 (Naples, Italy, 23-27 June 2025).

A-650. R. Merkle, C. Berger, A. Chesnokov, D. Gryaznov, E.A. Kotomin, J. Maier. "Mobile protons in triple-conducting perovskites - similarities and differences to electrolyte materials". INV.R.

A-651. R. Merkle, A. Chesnokov, D. Gryaznov, E. Bucher, E.A. Kotomin, J. Maier, W. Sitte. "The electronic structure, phase formation, and defect distribution in the Ba(Ce,Fe,Acc)O3 system investigated by density functional theory calculation". OR.

International Workshop on the Defect-Chemical Nature of Solids Petite-XIII (Bad Aibling, Germany, 9-12 September 2025).

A-652. D. Gryaznov, A. Chesnokov, E. Kotomin, R. Merkle. "Electronic structure and defect-proton interactions in triple-conducting perovskites: insights from DFT". OR.

22nd International Conference on Solid-State Protonic Conductors SSPC-22 (Copenhagen, Denmark, 14-19 September, 2025).

A-653. E. Bucher, C. Nader, A. Chesnokov, D. Gryaznov, R. Merkle, E.A. Kotomin, J. Maier, W. Sitte. "Triple-conducting Ba(Ce,Fe,Acc)O3- composites: phase formation, defect distribution and electronic structure". OR.

A-654. A. Chesnokov, D. Grayznov, E.A. Kotomin, R. Merkle. "Proton migration in doped and undoped BaFeO3: insights from DFT calculations". OR.

International Conference on Functional Materials and Nanotechnologies FMNT-2026 (Riga, Latvia, 15-18 June, 2026).

A-655. E.A. Kotomin et al. "First principles computer modelling of advanced materials for fusion applications". OR.

A-656. L.L. Rusevich, E.A. Kotomin, M.G. Brik. "First principles study of Mg2TiO4 inverse spinel: Critical comparison of pure and Mn4+ doped materials". PR.

A-657. G. Zvejnieks, E.Kotomin, L.Rusevich. "Bismuth modified SrTiO3 perovskites for green hydrogen production: DFT studies". PR.

A-658. I. Chevyakov, E.Kotomin, L.Rusevich. "Computational study of the structural, electronic, vibrational and elastic properties of Na2SiF6 and Na2SiF6:Mn4+ phosphors". PR.

A-659. V.N. Kuzovkov, E.Kotomin. "The effective diffusion coefficient in inhomogeneous solids with inclusions. A comparison of 2D continues and discrete models". PR.

International Congress on Sustainable Energy and related Technologies (ICSET 2026, Palermo, Italy).

A-660. E.Kotomin, G.Zvejnieks, L. Rusevich, N. Daneu, M.Krz'manc, A.Brunetti. First principles calculations of SrTiO3 engineering with Bi based heterostructures for efficient photostimulated hydrogen production. OR.

A-661. Yu.Mastrikov, D.Gryaznov, G.Zvejnieks, E.Kotomin. Density functional theory calculations on CeN4/SrTiO3 heterostructure. Ibid. OR