

Eugene KOTOMIN



Professor, Dr. habil. Phys., **Eugene KOTOMIN** (Jevgenijs Kotomins)
Head of Department for Theoretical Physics and Computer Modeling,
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Date and place of birth:

20 September 1949, Vilnius, Lithuanian Republic

Total citations 8600+

Citation H-index: 49

Number of papers in refereed journals: 510

Number of communications/posters at scientific meetings: 500+

Number of books and book chapters- 17, 12 review articles

Number of invited talks at International Conferences: 45

Main interests

Theoretical materials science based on first principles calculations

Theory of radiation-induced effects and defects in solids, kinetics of reactions with a focus on

Self-organization phenomena in diffusion-controlled reactions

Quantum chemistry of defective solids, nanomaterials and surfaces/interfaces

Current research activities are focused on

Functional materials and devices for new energy applications including solid oxide fuel cells, Li batteries, sensors

Nanomaterials and confinement effects in advanced perovskites

Defects and surface-related processes in advanced complex oxides and nitrides,

Physics and chemistry of actinides and nuclear fuels, new materials for fusion and fission reactors
Radiation physics and chemistry, self-organization in non-equilibrium systems

Honours

2011 Full member of the Latvian Academy of Sciences

2009 Corresponding member of the Latvian Academy of Sciences

1997 F. Cander's prize in Physics from Latvian Academy of Sciences

External expert for research project evaluations at the EC ERA-NET, Irish, Swiss, Estonian Universities, Scolkovo (Russian), as well as US Department of Energy (DOE), National Science Foundation (NSF) and PNNL laboratory.

Education (*degrees, dates, universities*)

- 1992 Dr habil. Phys., University of Latvia, Riga
- 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".
- 1975 Ph D 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"
- 1973-1974 Visiting Fellow, Dept. of Quantum Chemistry, Leningrad University. Advisor: Prof. R.A. Evarestov
- 1966-1971 B.S.+M.S. degrees: Dept. of Physics, Latvian State University, 19 Rainis blvd., Riga LV-1058, Latvia

Career/Employment (*employers, positions and dates*)

- 2008-2012- Visiting Professor, Astana University, Kazakhstan
- 1996-2000 Full Professor of the University of Latvia
- 2005-2007- Visiting Professor, EC Institute for Transuranium Elements, Karlsruhe, Germany
- 2001-2020- Visiting Scientist, Max Planck Institute for solid state research, Stuttgart, Germany
- 2000- DAAD Professor, Osnabrueck University, Germany
- 1998- DFG Professor, Osnabrueck University, Germany
- 1995- Visiting Professor, Aarhus University, Denmark
- 1988-present Leading Research Scientist and head of the theoretical laboratory at the Institute of Solid State Physics, The University of Latvia, Riga
- 1987-1991, A lecturer in general physics, University of Latvia, Riga
- 1987 Associate Professor, Dept. of Semiconductor Physics, Latvian State University
- 1986 Senior Visiting Fellow, Dept. of Theoretical Chemistry, Turin University, Italy. Advisor: Prof. C.Pisani
- 1980-1985 Scientist and Senior Scientist at the Institute of Solid State Physics
- 1975-1979 Assistant Professor, Dept. of Semiconductor Physics, Latvian State University, Riga
- 8 Kengaraga Str., LV-1063, Riga, Latvia
- 1971-1974 Engineer and Research Associate, Institute of Solid State Physics, Latvian State University,

Member of the organizing committees of the following International conferences:

Co-director of the NATO schools on computational chemistry, Italy, September 2001 and Radiation Physics, Erice, Italy, July 2004

NATO Advanced Research Workshop on Defects and Surface-Induced Effects in Advanced Perovskites, Riga, 1999

European Materials Research Society Meetings, Strasburg: 1993, 1994, 1995, 2014, 2016, 2017, 2018

Radiation Effects in Insulators (REI): since 1995 up to now (9 meetings)

Research support and agency

2019-2022 EC COST Action CA18234 Computational materials sciences for efficient water splitting with nanocrystals from abundant elements
2019-2022 ERA-NET project Sun2Chem on water splitting improvement on perovskite nanoparticles
2016-2018 ERA-NET project HarvEnPiez on piezoelectric properties of nano-perovskites
2015-2022 EUROFUSION project on Functional materials (WP-15-PPPT-MAT) for fusion applications
2014-2017 EC FP7 project GREEN-CC on ceramic membranes for gas separation
2012-2016 EC COST Action CM1104 on chemistry of oxides of reducible oxides
2006-2010 3 service contracts with the EC JRC Institute for Transuranium Elements, Karlsruhe, Germany
2009-2011 EC FP7 project NASA-OTM on innovation of new ceramic permeation membranes
2008-2011 EC FP7 project F-Bridge on development of new generation of nuclear fuels
2004-2006 NSF collaborative grant at Northwestern University, USA
1999-2000 Swedish-Latvian Joint research grant with Uppsala University
1999-2000 British-Latvian UK Royal Society Joint grant (University College London)
1999-2000 NATO research grant for senior visitors (Aarhus University, Denmark)
1996-1998 Volkswagen research grant Freie Universitat Berlin, Germany
1994-96 European Community HCM Network Grant on Large Scale Computer Simulations of Solids
1994-96 European Community Human Capital and Mobility (HCM) Network Grant on Polarons and Bipolarons in New Materials
1994-96 Two-year ISF research grant
1993, 1994, 1997 ISF travel grants for conferences
1992 International Science Foundation (ISF) grant

Recent selected publications

Books

1. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M.M. Kuklja, and J. Maier, Energy Conversion: Solid Oxide Fuel Cells. First-Principles Modeling of Elementary Processes. - Chapter 6 in book: Computational Approaches to Energy Materials (eds. A.Walsch, A.Sokol, C.R.A. Catlow, Wiley), 2013, p. 149-186.
2. Heifets E., Kotomin E.A., Mastrikov Yu., Piskunov S., and Maier J. Book chapter on Thermodynamics of ABO_3 perovskite surfaces. -- In: *Thermodynamics-Intective study* (InTech Open Access Publishers), 2012, p.491-518.
3. 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.—Book chapter 11 in: *Advances in Materials Science Research*, vol. 2, 2011, pp. 191-216 (Nova Science Publishers, ed. Maryann C. Wythers).
4. Sickafus K. and Kotomin E.A. (eds.). Radiation Effects in Solids, 2006, NATO ASI Science Series II. Physics, Chemistry and Mathematics, Vol. **235**.
5. 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**).
6. 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.
7. 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. -320 p.
8. Evarestov R.A., Kotomin E.A., Ermoshkin A.N. Molecular models of point defects in wide-gap solids. -Riga: Zinatne, 1983. -287 p.

Review Articles

1. 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**, p. 5443-5471.
2. 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 2006* (Eds. K. Sickafus and E.A. Kotomin), **235**, p. 153-192.
3. 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.
4. Eglitis R., Kotomin E.A., Borstel G. Large scale computer modeling of point defects, polarons and perovskite solid solutions. – *Defects and Diffusion Forum*, 2004, **226-228**, p. 169-180.
5. 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.
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. 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.
8. 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.
9. 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.
10. 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.
11. 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.

Publications

1. 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.
2. R.A. Evarestov, A. Senocrate, E.A. Kotomin, J. Maier. First-principles calculations of iodine-related point defects in CsPbI₃. *Phys. Chem. Chem. Phys.*, 2019, **21**, pp. 7841-7846
3. L.L. Rusevich, G. Zvejnieks, E.A. Kotomin. Ab initio simulation of (Ba,Sr)TiO₃ and (Ba,Ca)TiO₃ perovskite solid solutions.-- *Solid State Ionics*, 2019, **337**, pp. 76–81.
4. A.Platonenko, D. Gryaznov, Yu.F. Zhukovskii, E.A. Kotomin. First principles simulations on migration paths of oxygen interstitials in MgAl₂O₄. *Phys. Stat. Solidi B*, 2019, **256**, 1800282 (pp. 1-7).
5. 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)
6. N. Sobolev, F. Djurabekova, E.A. Kotomin. Defect-induced effects in nanomaterials. --- *Phys. Status Solidi B*, 2019, **256**, 1900181 (pp. 1-2)
7. A.Chesnokov, D. Gryaznov, E.A. Kotomin. First principles calculations on CeO₂ doped with Tb³⁺ ions. *Optical Materials*, 2019, **90**, 76-83.
8. E. Heifets, E. A. Kotomin, A. A. Bagaturyants, J. Maier. Thermodynamic stability of non-stoichiometric SrFeO₃: a hybrid DFT study. *Chem. Phys. Phys. Chem.* 2019, **21**, 3918.
9. L.L. Rusevich, G. Zvejnieks, E.A. Kotomin, M. Macek Krzmann, A. Meden, S. Kunej, I.D. Vlaicu. Theoretical and experimental study of (Ba,Sr)TiO₃ perovskite solid solutions and BaTiO₃/SrTiO₃ heterostructures. *J. Phys. Chem. C*, 2019, **123**, pp. 2031–2036.
10. 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).

11. 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).
12. 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. 258–264
13. 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. (1-7).
14. 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)
15. Yu.A. Mastrikov, M.N. Sokolov, S. Koch, Yu.F. Zhukovskii, A. Gopejenko, P.V. Vladimirov, V.A. Borodin, E.A. Kotomin, and A. Möslang. Ab initio modelling of the initial stages of the ODS particle formation process. *Nucl. Instrum. Methods Phys. Res. B*, 2018, 435, pp. 70–73.
16. A. Platonenko, D. Gryaznov, Yu.F. Zhukovskii, and E.A. Kotomin. Ab initio simulations on charged interstitial oxygen migration in corundum. *Nucl. Instr. Methods Phys. Res. B*, 2018, 435, pp. 74–78.
17. V.N. Kuzovkov, E.A. Kotomin, and A.I. Popov. Kinetics of dimer F₂ type center annealing in MgF₂ crystals. *Nucl. Instrum. Methods Phys. Res. B*, 2018, 435, pp. 79–82
18. G.A. Kaptagay, Yu.A. Mastrikov, and E.A. Kotomin. First-principles modelling of N-doped Co₃O₄. *Latv. J. Phys. Tech. Sci.*, 2018, 55, Nr 5, pp. 36-42
19. M.F. Hoedl, E. Makagon, I. Lubomirsky, R. Merkle, E.A. Kotomin, and J. Maier. Impact of point defects on the elastic properties of BaZrO₃: comprehensive insight from experiments and ab initio calculations. *Acta Mater.*, 2018, 160, pp. 247-256.
20. 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.
21. 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.
22. 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 Al₂O₃ single crystals. *Nucl. Instrum. Methods Phys. Res. B*, 2018, 433, pp. 93-97.
23. G. Zvejnieks, A. Anspoks, E.A. Kotomin, and V.N. Kuzovkov. Kinetic Monte Carlo modeling of Y₂O₃ nano-cluster formation in radiation resistant matrices. *Nucl. Instrum. Methods Phys. Res. B*, 2018, 434, pp. 13-22.
24. 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. 28–32
25. V.N. Kuzovkov, E.A. Kotomin, and A.I. Popov. Kinetics of the electronic center annealing in Al₂O₃ crystals. *J. Nucl. Mater.*, 2018, 502, pp. 295-300.

Reviewer for more than 40 basic research journals, including

Physical Review Letters, Physical Review B and E, Nature Materials, Journal of Nuclear Materials, Nuclear Instruments and Methods B, J. Applied Physics, Solid State Ionics, Surface Science, Applied Surface Science, Physical Chemistry Chemical Physics, Physica Status Solidi, Physica B, J Luminescence, Chemistry of Materials, J Physical Chemistry, J. Physical Chemistry Letters, J Physics: Condensed Matter, Solid State Communications, Chemical Physics, Philos. Magazin, Applied Physics Letters, J. Materials Chemistry, Advanced Materials, Advanced Functional materials, Chemical Physics Letters, Computational Materials Science, Radiation Effects and Defects in Solids, J. Alloys and Compounds, Energy and Environmental Science.