

# **JEVGĒNIJA KOTOMINA ZINĀTNISKĀ BIOGRĀFIJA**

## **(CURRICULUM VITAE)**

<http://teor.cfi.lu.lv/index.php?slab=staff>

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**ZINĀTNISKAIS GRĀDS:** Dr. habil. fizikā, <https://orcid.org/0000-0002-8122-6276>

LZA īstena loceklis

**DZIMŠANAS DATUMS UN VIETA:** 1949. g. 20. septembris, Viļņa, Lietuva.

**PERSONAS KODS:** 200949-10900

**ADRESE:** Latvijas Universitātes Cietvielu fizikas institūts (CFI), Ķengaraga iela 8, LV-1063 Rīga.

**Mājas adrese:** Rupniecības 17-12, Rīga LV-1010

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**ĢIMENES STĀVOKLIS:** precējies, divi bērni.

### **IZGLĪTĪBA**

- 1992 Dr. habil. phys., Latvijas Universitāte, Rīga.
- 1988 Zinātņu doktora grāds cietvielu fizikā.  
Tēma: "Elektronu tunelēšanās kontrolētā defektu akumulācijas un rekombinācijas teorija jonu kristālos".
- 1975 Zinātņu kandidāta grāds: Fizikas institūts, Latvijas Zinātņu akadēmija. Vadītājs: Prof. I. Tāle  
Tēma: "Elektronu tunelēšanās loma radiācijas-inducēto defektu akumulācijā un defektu difūzijas-kontrolētās reakcijās. "
- 1973-1974 Vieszinātnieks, Kvantu ķīmijas fakultāte, Ļeņingradas Universitāte. Vadītājs: Prof. R.A. Evarestovs
- 1966-1971 B.S.+M.S. grāds: Fizikas fakultāte, Latvijas Valsts Universitāte, Raiņa bulv. 19, Rīga LV-1058, Latvija

### **AKADEMISKĀ UN PROFESSIONĀLĀ PIEREDZE**

- 2011 LZA akadēmiķis
- 2009 LZA korespondētājloceklis
- 1988-līdz šim brīdim, Vadošais pētnieks un Teorētiskās fizikas un datormodelēšanas nodaļas vadītājs LU Cietvielu fizikas institūtā.
- 1987-1991, Lektors vispārīgā fizikā, Latvijas Universitāte, Rīga.
- 1987 Asociētais Profesors, Pusvadītāju fizikas nodaļa, LVU, Rīga.
- 1986 Vecākais vieszinātnieks, Teorētiskās ķīmijas fakultāte, Turīnas Universitāte, Itālija. Vadītājs: Prof. C.Pisani.
- 1980-1985 Pētnieks un vadošais pētnieks, Cietvielu fizikas institūts, LVU, Rīga.
- 1975-1979 Profesora asistents, Pusvadītāju fizikas katedra, LVU, Rīga. Ķengaraga 8, LV-1063, Rīga, Latvija.
- 1971-1974 Inženieris, Cietvielu fizikas institūts, Latvijas Valsts Universitāte (LVU),

## BALVAS

1997 F. Candra Latvijas Zinātņu akadēmijas balva fizikā

## GALVENĀS ZINĀTNISKĀS INTERESES:

### Cietvielu kvantu ķīmija (*jauns zinātnes virziens Latvijā*)

#### Skaitļošanas (*ab initio*) metodes materiālzinātnē

Nanomateriālu teorija

Jauni materiāli enerģētikai

Radiācijas fizika un ķīmija

Cietvielu defektu teorija

Virsmas zinātne, katalīze un virsmas reaktivitāte

Citešanas: 8900, H-indeks 50

## ZINĀTNISKĀS PUBLIKĀCIJAS

Publikāciju skaits referējamos žurnālos: 490

Ieguldījums zinātniskajās konferencēs: 520

Grāmatu un monogrāfiju daļas skaits: 17, 12 apskati,

45 ielūgtie referāti starptautiskās konferencēs

## Jaunākas publikācijas

1. D. Zablotzky, L.L. Rusevich, G. Zvejnieks, V. Kuzovkov, E. Kotomin. Manifestation of 1dipole-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 CsPbI<sub>3</sub>. *Phys. Chem. Chem. Phys.*, 2019, 21, pp. 7841-7846
3. L.L. Rusevich, G. Zvejnieks, E.A. Kotomin. Ab initio simulation of (Ba,Sr)TiO<sub>3</sub> and (Ba,Ca)TiO<sub>3</sub> 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 MgAl<sub>2</sub>O<sub>4</sub>. *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 CeO<sub>2</sub> doped with Tb<sup>3+</sup> ions. *Optical Materials*, 2019, 90, 76-83.
8. E. Heifets, E. A. Kotomin, A. A. Bagaturyants, J. Maier. Thermodynamic stability of non-stoichiometric SrFeO<sub>3</sub>: 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)TiO<sub>3</sub> perovskite solid solutions and BaTiO<sub>3</sub>/SrTiO<sub>3</sub> 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 Co<sub>3</sub>O<sub>4</sub> 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 MgAl<sub>2</sub>O<sub>4</sub>. *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 F<sub>2</sub> type center annealing in MgF<sub>2</sub> 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 Co<sub>3</sub>O<sub>4</sub>. *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 BaZrO<sub>3</sub>: 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 Al<sub>2</sub>O<sub>3</sub> single crystals. *Nucl. Instrum. Methods Phys. Res. B*, 2018, {bf 433}, pp. 93-97.
23. G. Zvejnieks, A. Anspoks, E.A. Kotomin, and V.N. Kuzovkov. Kinetic Monte Carlo modeling of Y<sub>2</sub>O<sub>3</sub> 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 Al<sub>2</sub>O<sub>3</sub> crystals. *J. Nucl. Mater.*, 2018, 502, pp. 295-300.

## Grāmatas

1. Sickafus K. and Kotomin E.A. (eds.). *Radiation Effects in Solids*, 2006, NATO ASI Science Series II. Physics, Chemistry and Mathematics, Vol. **235**.
2. 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**).
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 *Comprehensive Chemical Kinetics*), 1996. 620 p.
4. 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 (krievu val.), 1991. -320 p.
5. Evarestov R.A., Kotomin E.A., Ermoshkin A.N. *Molecular models of point defects in wide-gap solids*. -Riga: Zinātne (krievu val.), 1983. -287 p.

## Monogrāfiju daļas

6. 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.
7. 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.
8. 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).

## Apskati

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 (Eds. K. Sikafus and E.A. Kotomin), 2006, **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.

## Starptautisko konferenču organizācijas komitejas loceklis:

- Ceramic Membranes for Energetics, Riga, 2011
- 2x NATO skolu direktors: Computational chemistry, Il Cicco, Italy, September 2001; 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 Meeting, Strasburg, 1995,
- 9x Radiation Effects in Insulators (REI): Catania, 1995; Tennessee, 1997; Jena, 1999, Lisbon, 2001, Brasil, 2003; Santa Fe, USA, 2005, Caen, France, 2007, Padova, Italy, 2009, Beijing 2011, Versaile 29'017, Astana 2019.
- Quantum Chemistry of Solids; Riga 1985, 1990

### **Ielūgtie referāti starptautiskās konferencēs:**

- The 18th Israel Materials Engineering Conference IMEC-18 (Dead Sea, Israel, February 2018)
- European Conference on defects in Insulating Materials (EURODIM), (Bydgoszcz, Poland, 8-13 July 2018).
- 21st International Conference on Solid State Ionics, Padua, Italy, 2017
- 232st Electrochemical Society Meeting, New Orleans, USA, 2017
- Schools-conferences on "Atomistic Simulations of Functional Materials" (Moscow, Russia, 2014-2018)
- Materials Science and technology (USA) Pittsburg, 2009
- Intern. Conference on Radiation Physics and Chemistry of Inorganic Materials, Astana, 2009
- Intern. Workshop on Fundamentals of Li-based Batteries, Tegersee, Germany, November 2008
- Intern. Workshop on *ab initio* simulations of crystalline solids, Torino, Italy, September 2008
- 5. Baltic Conference on Electrochemistry, Tartu, May 2008
- Baltic Conferences on Functional Materials and Nanotechnology, Riga, 2008-2011
- XNO workshop on nuclear fuels modelling, Tokyo, February 2008
- 2 lectures at NATO school on Radiation Physics, Erice, Italy, July 2004
- Electronic Structure: Principles and Applications (ESPA-2004), Valladolid, Spain, September 2004
- 10th International Ceramic Congress, Florence, 2002
- NATO ARW on Atomistic Aspects of Epitaxial Growth, Corfu, 2001
- European Materials Research Society Meetings, Strasburg, 1995, 1999
- 12 Nordic Symposium on Computer Simulations, Finland, 1998
- 1st ABS International Symposium on Metal Oxide Surfaces, Tsukuba, Japan, 1998
- Advanced Optical Materials and Devices, Riga, Latvia, 1996
- 2nd Intern. Conference on Excitonic Processes in Condensed Matter, Gohrisch, Germany, 1996
- Defects in Insulating Materials (ICDIM), Winston-Salem, 1996, Johannesburg, 2000
- NATO Advanced Research Workshop on Computer Modelling of Processes in Solids, Wroclaw, 1996
- Radiation Effects in Insulators, Nagoya, 1994, Knoxville, 1997; Caen 2007

### **Projektu vadība:**

- 2019-2022 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 SunToChem on Engineering of perovskite photocatalysts for sunlight-driven hydrogen evolution from water splitting
- 2018-2019 Bilateral Latvia-Ukraine project on perovskite surface reactivity
- 2016-2019 M-ERA-NET project HarvEnPiez on Innovative nano-materials and architectures for integrated piezoelectric energy harvesting applications
- 2015-2020 Eurofusion project on Functional optical materials
- 2015-2017 Eurofusion Enabling Research Project on X-ray Absorption Spectroscopy and atomic-scale modelling of ODS steels
- 2014-2018 Russian Science Foundation project 14-43-00052 on large scale advanced materials modelling
- 2014-2017 EC FP7 project GREEN-CC on ceramic membranes for gas separation
- 2012-2016 EC COST project CM1104 on chemistry of oxides of reducible oxides
- 2009-2011 EC FP7 project NASA on innovation of new ceramic membranes for gas separation
- 2008-2010 EC FP7 project F-Bridge on development on new generation of nuclear fuels
- 2006-2010 3 service contracts with EC Institute for Transuranium Elements, Karlsruhe, Germany
- 2004-2008 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

### **Ielūgtais eksperts**

- ASV Enerģētikas Departamenta (Department of Energy, DOE) Nacionālās Zinātnes Fonda (National Science Foundation, NSF) un PNNL laboratorijas projektiem; kā arī
- Skolkovo (Krievija), Igaunija, Īrija, Izraēla, Ungārija, ERA-NET projektiem

### **Recenzents 40 vadošos starptautiskajos žurnālos:**

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, u.t.t.

Paraksts

/J.Kotomins/

Datums 2019.gada 5.jūlijā