



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 īstenais loceklis

DZIMŠANAS DATUMS UN VIETA: 1949. g. 20. septembrī, 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

Pedagoģiskais darbs: vadīti 20 bakalaura darbi, 15 maģistra darbi, 8 promocijas darbi. Lekciju kursi par modernu materiālu datormodelēšanu Astanas Universitātē (Kazahstana), Maksa Planka institūtā (Stutgarte, Vācija). Ielūgtais DAAD un DFG profesors Vācijā.

Citešanas: 11.000+, H-indeks 53

Saskaņā ar vadošās akadēmiskās pētniecības platformas "research.com" 2023. gada datiem, <https://research.com/scientists-rankings/chemistry/ly>, J.Kotomins ir ierindojies pirmajā vietā Latvijā (teorētiskās) ķīmijas jomā.

ZINĀTNISKĀS PUBLIKĀCIJAS

Publikāciju skaits referējamos žurnālos: 470

Ieguldījums zinātniskajās konferencēs: 520

Grāmatu un monogrāfiju daļas skaits: 17, 12 apskati,

45 ielūgtie referāti starptautiskās konferencēs

Jaunākas publikācijas (5 gadi)

1. G. Lee, Y.-C. Cheng, Y.-T. Lin, J.C.S. Wu, W.-Y. Yu, M. Maček Kržmanc, S. Gupta, E.A. Kotomin. Photocatalytic water splitting of Al-doped $Rh_xCr_{2-x}O_3/SrTiO_3$ synthesized by flux method: Elucidating the role of different molten salts.--- J. Phys. Chem. C, 2023, 127, pp. 9981–9991.
2. 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 $SrTiO_3$.-- Adv. Theory Simul., 2023, 2200619 (pp. 1-7). **Open Access**
3. Y.-Y. Tai, J.C.S. Wu, W.-Y. Yu, M. Maček Kržmanc, E.A. Kotomin. Photocatalytic water splitting of improved strontium titanate for simultaneous separation of H_2 in a twin photoreactor.--- Appl. Catal. B, 2023, 324, 122183 (pp. 1-10).
4. L.L. Rusevich, E.A. Kotomin, G. Zvejnieks, M. Maček Kržmanc, S. Gupta, N. Daneu, J.C.S. Wu, Y.-G. Lee, W.-Y. Yu. The Effects of Al doping on hydrogen production efficiency upon photostimulated water splitting on $SrTiO_3$ nanoparticles.--- J. Phys. Chem. C, 2022, 126, pp. 21223–21233.
5. V. Krasnenko, L.L. Rusevich, A. Platonenko, Yu.A. Mastrikov, M. Sokolov, E.A. Kotomin. Water splitting on multifaceted $SrTiO_3$ nanocrystals: calculations of Raman vibrational spectrum. Materials, 2022, 15, 4233 (pp. 1-17). **Open Access**
6. L.L. Rusevich, M. Tyunina, E.A. Kotomin, N. Nepomniashchaia, A. Dejneka. The electronic properties of $SrTiO_{3-\delta}$ with oxygen vacancies or substitutions.--- Sci. Rep., 2021, 11, 23341 (pp. 1-8). **Open Access**
7. M. Sokolov, Yu.A. Mastrikov, G. Zvejnieks, D. Bocharov, E.A. Kotomin, V. Krasnenko. Water splitting on multifaceted $SrTiO_3$ nanocrystals: computational study.---Catalysts, 2021, 11, 1326 (pp. 1-8). **Open Access**
8. 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.
9. D. Zablotsky, 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.
10. 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
11. 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. 76–81.
12. A. Platonenko, D. Gryaznov, Yu.F. Zhukovskii, E.A. Kotomin. First principles simulations on migration paths of oxygen interstitials in $MgAl_2O_4$. Phys. Stat. Solidi B, 2019, 256, 1800282 (pp. 1-7).
13. 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)
14. N. Sobolev, F. Djurabekova, E.A. Kotomin. Defect-induced effects in nanomaterials. --- Phys. Status Solidi B, 2019, 256, 1900181 (pp. 1-2)
15. A. Chesnokov, D. Gryaznov, E.A. Kotomin. First principles calculations on CeO_2 doped with Tb^{3+} ions. Optical Materials, 2019, 90, 76-83.
16. 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.

- 17 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.
- 18 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 catalytic activity. *J. Phys.: Conf. Ser.*, 2018, 1115, 032032 (pp.1-6).
- 19 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).
- 20 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
- 21 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).
- 22 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)
- 23 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.
- 24 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.
- 25 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.
- 26 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.

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 ABO₃ perovskite surfaces*. -- In: *Thermodynamics-Intelective 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 pervoskite 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,
- 9 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:

- 2020-2023 FLAG-ERA JTC project To2Dox (Transferable two-dimensional correlated oxide layers)
- 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 2023.gada 5.septembri