



## 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** 371-67-187-480 (office), 371-7-326308 (home)

**Fax** 371-6711-2583

**E-mail** kotomin@latnet.lv, <http://www.cfi.lu.lv/teor/index.html>, [www.lza.lv/scientists/kotomine.htm](http://www.lza.lv/scientists/kotomine.htm)

**Marital Status** Married, two children

**Total citation: 5050; H-index: 34;**  
**420 research papers (5 in PRL, 26 in PRB and PRE, 11 in Surface Science),**  
**12 review articles, author/editor of 12 books and book chapters**

## 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

- since October 2009** Corresponding Member of the Latvian Academy of Sciences
- 05-06.1989** Invited Professor, Inorganic Chemistry Dept., University of Turin, Italy
- 05.1990,** Visiting Scientist, University of Bayreuth, Germany
- 03.1991**
- 12.1990** Visiting Scientist, Ben-Gurion University, Israel

**09.91-02.1992;** CCP Fellow at the University of Western Ontario, Canada  
**03.1999**  
**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  
**08.2007-12.2013** Visiting Scientist at Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany  
**2005-2009** External evaluator of the DOE,NSF and PNNL research projects: 2005, 2007, 2009

**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)
- European Materials Research Society Meeting, Strasburg, 1995; Warsaw, 2012
- 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

**35 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
- 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
- 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
- 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
- Materials Science and Technology, USA, Pittsburg 2009, Columbus 2011
- International Conference on Defects in Insulating Materials (ICDIM) Santa Fe, June 2012
- Materials Research Society Meeting, San Francisco, 2013

#### **Member of the:**

- Full Member of the Latvian Academy of Sciences since 2011
- 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**

- |             |   |
|-------------|---|
| <b>1992</b> | International Science Foundation (ISF) grant  |
| <b>1992</b> | NATO collaborative grant on Defects in Oxides |

<b>1993,</b> <b>1994,1997</b>	ISF (Soros) travel grants for International conferences
<b>1994-96</b>	Two-year ISF research grant
<b>1994-96</b>	European Community Human Capital and Mobility (HCM) Network Grant on <i>Polarons and Bipolarons in New Materials</i>
<b>1994-96</b>	European Community HCM Network Grant on <i>Large Scale Computer Simulations of Solids</i>
<b>1996-98</b>	Volkswagen research grant (Freie Universität Berlin, Germany)
<b>1999-2000</b>	NATO research grant for senior visitors (Aarhus University, Denmark)
<b>1999-2000</b>	British-Latvian UK Royal Society Joint grant (University College London)
<b>1999-2003</b>	Swedish-Latvian Joint research grants with Uppsala University
<b>2001-2004</b>	Networking grant in the framework of the EC Excellence Center for Materials Research and Technology, CAMART
<b>2001-2003</b>	NATO collaborative grant on Defects in Perovskites, Osnabrueck University, Germany
<b>2003-2006</b>	Research grant of German-Israeli Foundation: MPI,Stuttgart– Technion, Israel
<b>2002-2005</b>	Member of the European Network Psi-k2 on Atomistic Materials Design
<b>2005-2007</b>	NSF collaborative grant on Reactivity of Oxide Surfaces with NRSEC Northwestern University, USA
<b>2005-2007;</b> <b>2010-2012</b>	Two projects of the German-Israel Foundation (GIF) on new materials for solid oxide fuel cells
<b>2006-2010</b>	Three service contracts on ab initio modelling of nuclear fuels with JRC-ITU, Karlsruhe, Germany
<b>2006-2014</b>	Euratom-Latvia project on modeling of ODS steel formation as reactor materials, Brussels, Belgium
<b>2007-2008</b>	Actinet: EC Euratom Network on He modelling in nuclear fuels
<b>2008-2011</b>	EC FP7 Project F-Bridge on nuclear fuel modelling
<b>2009-2012</b>	EC FP7 Project NASA on ceramic membrane modelling for gas separation
<b>2008-20012</b>	ERANET project MATERA on materials for resistive switching
<b>2010-2013</b>	Research grant of German-Israeli Foundation: MPI,Stuttgart– Technion, Israel

**2013-2017** EC FP7 Project GREEN on advanced ceramic membranes

**2002-2015** EC COST Project CM1104 on catalytic materials with variable oxidation states

## **AWARDS**

**1997** Fridrich Candere's prize in physics of the Latvian Academy of Sciences

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, 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 in Astana Eurasian University (Kazakhstan) on "Computational Methods and Modelling of Advanced Materials".

I have supervised 20 BS theses, 15 MS theses and 6 PhD theses, at the University of Latvia and Max Planck Institute in Stuttgart, Germany.

## **PUBLICATIONS**

Author/co-author of 12 books and chapters, 12 review articles, 420 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 solid oxide fuel cells (SOFC), Li 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 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'), Northwestern University, Evanston, USA (Prof. D. Ellis, M.O. de la Cruz, 'Reactivity of Surfaces and Self-Assembling'), University of Maryland (Prof. M. Kuklja, 'First-principles modeling of Solid Oxide Fuel Cells'), Idaho National Laboratory (Dr S.Rashkeev, 'Computer simulations of nuclear fuels'), Turin University, Italy (Prof. R. Dovesi, 'LCAO hybrid Calculations of Solids, Surfaces and Interfaces'), University of Aarhus, Denmark (Prof. N.E. Christensen, 'The Atomic and Electronic Structure of Solids and Defects'), Center of Nanotechnology, University Colledge London, UK (Prof. A.L.Shluger, 'Reducible oxide surfaces'), Ben-Gurion University, Israel (Prof. D.Fuks, 'Perovskite solid solutions'), 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').

**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., Zvejniaks 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<sub>3</sub> 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 Access 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 1 of the Fall EMRS conference (Warsaw, 2012)– Phys. Stat. Solidi B 250, No 4, 2013.

**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 perovskite 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 describing 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., Valdat's 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. Rigorous 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 thallos 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  $A + B \rightarrow B$  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<sub>2</sub> 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 TiCl 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]<sup>0</sup> 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.



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.

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.512-515.

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. 5901-5910.

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  $\alpha$ - $Al_2O_3$  Crystals. - Phys. Rev. Lett., 1992, **69**, p.1411-1414.

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 diffusion-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  $A + B \rightarrow 0$  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  $A + B \rightarrow 0$  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<sub>2</sub>O. - 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<sub>x</sub>Br<sub>1-x</sub> 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  $A + B \rightarrow 0$  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  $A + B \rightarrow 0$  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  $A + B \rightarrow B$  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<sub>2</sub> 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  $\text{KNbO}_3$ , *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  $\text{MgO}$  and  $\alpha - \text{Al}_2\text{O}_3$  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  $\text{BaTiO}_3$ . - *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  $\text{KCl}$  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  $\text{MgO}$  . - *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  $\alpha - \text{Al}_2\text{O}_3$  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  $\text{KNbO}_3$ . - *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  $\text{KNbO}_3$  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  $\text{KNbO}_3$  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  $\text{KNbO}_3$  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)*



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  $A + B \rightarrow B$  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  $A + B \rightarrow 0$  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<sub>3</sub>: *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<sub>2</sub> 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<sub>2</sub>O<sub>3</sub> (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<sub>2</sub> 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<sub>3</sub> (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<sub>3</sub> . 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<sub>3</sub> 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<sub>3</sub> and Li impurity in KTaO<sub>3</sub>. 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<sub>3</sub> 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<sub>3</sub>, LiNbO<sub>3</sub> and KTiPO<sub>4</sub>. - 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<sup>-</sup> 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  $\text{KNbO}_3$  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  $\text{KNbO}_3$ . - *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 hydrate ion in  $\text{MgO}$  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  $\text{Ag/MgO}$  (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  $\text{KNbO}_3$ . - *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  $\text{KNbO}_3$  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  $\text{KNbO}_3$  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  $\text{MgO}$  (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  $\text{KNbO}_3$  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  $\text{F}^+$  Centers in Neutron- Irradiated  $\text{MgO}$ . - *Ibid.*, p. 220-224.

225. Kotomin E.A., Heifets E. Atomistic Simulation of  $\text{SrTiO}_3$  and  $\text{BaTiO}_3$  (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<sub>3</sub> (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<sub>3</sub> 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<sub>3</sub> 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<sub>3</sub> 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<sub>3</sub> 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<sub>2</sub>O<sub>3</sub> (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<sub>3</sub> 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<sub>3</sub>. - *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<sub>3</sub> 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<sub>3</sub> 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<sub>3</sub>. - *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<sub>3</sub> 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<sub>3</sub> 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<sub>3</sub> 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<sub>3</sub> 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<sub>3</sub> (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<sub>3</sub> (100) Surface Structure. – In: *Proc. Williamsburg Meeting on Fundamental 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<sub>3</sub> (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<sub>3</sub>. – *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<sub>3</sub>. – 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<sub>3</sub> (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, Strasbourg, 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 Processing, 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, Kapphann S.E., and Vikhnin V.S. Semi-empirical

- Calculations of the Electronic and Atomic Structure of Polarons and Excitons in ABO<sub>3</sub> 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<sub>3</sub> (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 Retrospective 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<sub>3</sub> 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<sub>3</sub> 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<sub>3</sub> (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<sub>3</sub> 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  $\text{KNbO}_3$  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  $\text{ABO}_3$  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  $\text{SrTiO}_3$ ,  $\text{BaTiO}_3$  and  $\text{PbTiO}_3$  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  $\text{LaMnO}_3$  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  $\text{LaMnO}_3$  and  $\text{SrMnO}_3$ . – 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  $\text{SrZrO}_3$  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  $\text{ABO}_3$  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  $\text{SrTiO}_3$  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  $\text{ABO}_3$  perovskite (001) surface.– Cond. Matter Arxiv, cond.mat/0405463

319. Fuks D., Dorfman S., Piskunov S., and Kotomin E.A. Ab initio Thermodynamics of  $\text{BaSrTiO}_3$  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  $\text{AgCl}(111)$  surface and  $\text{AgCl}(111)/\text{Al}_2\text{O}_3$  (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  $\text{Ba}_{0.5}\text{Sr}_{0.5}\text{TiO}_3$  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  $\text{LaMnO}_3$  (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  $(\text{BaSr})\text{TiO}_3$  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  $\text{LaMnO}_3$  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  $\text{ABO}_3$  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  $\text{BaTiO}_3$  (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  $\text{SrTiO}_3$ ,  $\text{BaTiO}_3$ , and  $\text{PbTiO}_3$  (001) surfaces: *Ab initio* DFT/HF hybrid calculations. - ibid, 2005, p. 472-477.

329. Piskunov S., Dorfman S., Fuks D., and E.A. Kotomin,  $\text{BaSr}_{1-c}\text{TiO}_3$  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  $\text{LaMnO}_3$  (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  $\text{AgCl}(111)$  surface and  $\text{AgCl}(111)/\text{a-Al}_2\text{O}_3(0001)$  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  $\text{Ba}_{0.5}\text{Sr}_{0.5}\text{TiO}_3$  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  $\text{Ba}_{0.5}\text{Sr}_{0.5}\text{TiO}_3$  heterostructure: *ab initio* hybrid density functional calculations. - Phys. Scripta (Proc. Int. Meeting on Applied Physics, Badajoz, 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<sub>3</sub>. - 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., Hoeffft 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<sub>3</sub> 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<sub>3</sub> 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<sub>3</sub> (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 LaSr<sub>1-x</sub>MnO<sub>3</sub> 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<sub>3</sub>. - 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<sub>3</sub> (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.



349. Heifets E., Piskunov S., Kotomin E.A., Zhukovskii Yu.F., and Ellis D.E. Electronic structure and thermodynamic stability of double-layered SrTiO<sub>3</sub> (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<sub>3</sub> 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<sub>3</sub> 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<sub>3</sub> 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 nanocomposites: 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<sub>2</sub>O. - 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<sub>3</sub> (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<sub>3</sub> (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<sub>3</sub> 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<sub>3</sub>. - 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<sub>2</sub>-terminated (001) surfaces of cubic PbZrO<sub>3</sub>: 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<sub>3</sub> 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<sub>3</sub> crystals. – J. Chem. Phys., 2008, **129**, 214704.

## 2009

369. Mastrikov Yu., Heifets E., Kotomin E.A., and Maier J. Atomic, electronic and thermodynamic properties of cubic and orthorhombic LaMnO<sub>3</sub> 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<sub>3</sub>, PbZrO<sub>3</sub> and SrTiO<sub>3</sub> 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. Zhukovskii 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 ABO<sub>3</sub> 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<sub>2</sub> 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<sub>3</sub> 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<sub>3</sub> 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<sub>3</sub>. – 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<sub>2</sub> (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<sub>3</sub>. – 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<sub>1-x</sub>Sr<sub>x</sub>)(Co<sub>1-y</sub>Fe<sub>y</sub>)O<sub>3</sub>- 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<sub>2</sub>: 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<sub>3</sub> 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<sub>2</sub> (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<sub>3</sub>: 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<sub>2</sub>O<sub>3</sub> 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<sub>3</sub> 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<sub>3</sub> 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 SrTiO<sub>3</sub>(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  $\alpha$ -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 Ba<sub>1-x</sub>Sr<sub>x</sub>Co<sub>1-y</sub>Fe<sub>y</sub>O<sub>3</sub> 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<sub>2</sub> 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<sub>3</sub> 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 spinorbital effects in uranium mononitride nuclear fuels. - *Phys. Chem. Chem. Phys.*, 2012, **14**, p. 44824490.

408. E. Blokhin, E.A. Kotomin, and J. Maier, First-principles phonon calculations of Fe<sup>4+</sup> impurity in SrTiO<sub>3</sub>. - 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, Disorder, and Structural Stability of Ba<sub>x</sub>Sr<sub>1-x</sub>Co<sub>y</sub>Fe<sub>1-y</sub>O<sub>3</sub> 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<sub>2</sub> 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 Journal 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<sub>1-x</sub>Sr<sub>x</sub>Co<sub>1-y</sub>Fe<sub>y</sub>O<sub>3</sub> perovskites: insight from ab initio calculations and comparison with Ba<sub>1-x</sub>Sr<sub>x</sub>Co<sub>1-y</sub>Fe<sub>y</sub>O<sub>3</sub>. - 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<sub>1-c</sub>,Sr<sub>c</sub>)CoO<sub>3</sub> solid solutions. - Solid State Ionics, 2013, **230**, p. 3236.
415. M.M. Kuklja, Yu.A. Mastrikov, B. Jansang, and E.A. Kotomin, First principles calculations of (Ba,Sr)(Co,Fe)O<sub>3</sub> structural stability. - Solid State Ionics, 2013, **230**, p. 2126.
416. Fuks D., Weizman A., and Kotomin E.A., Phase competition in (La,Sr) CoO<sub>3</sub> 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<sub>3</sub>. - 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<sub>2</sub> crystals. - Phys. Status Solidi C, 2013, **10**, p. 160164. (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. 102106.
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<sub>3</sub>: emphasis on phonon contribution. - J. Phys. Chem. C, 2013, **117**, p. 13776-13784.

## 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-temperature 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 structure 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  $A + B \rightarrow B$  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<sub>2</sub> and Li<sub>2</sub>SiO<sub>3</sub>. -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 Ex-citonic 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  $F^+ \rightarrow F$  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  $\text{KNbO}_3$  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  $\text{KNbO}_3$  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  $\alpha - \text{Al}_2\text{O}_3$  crystals. - Ibid., p. 152.
- A-105. Heifets E., Dorfman S., Fuks D., and Kotomin E. Atomic simulation of the (001) surface in  $\text{BaTiO}_3$ . - 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: effects 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<sup>+</sup> centers in KNbO<sub>3</sub> 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<sub>3</sub> crystals. - Abstr.4th Intern.MRS Conf.in Asia, Chiba, Japan, Sept. 1997, Symposium R, p.20

A-123. Heifets E., Zhukovskii Yu., and Kotomin E.A., Ab initio Hartree-Fock Simulations of Silver Film Adhesion on both A<sub>2</sub>O<sub>3</sub> (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<sub>2</sub> 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, Tennessee, 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 Ferroelectricity, 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<sub>3</sub> perovskites, Psik-2000 Conference on *em Ab initio* (from electronic structure) calculations of complex processes in Materials, Schwabisch 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<sub>3</sub> (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<sub>3</sub> 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<sub>3</sub> 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<sub>3</sub> 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<sub>3</sub>. *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 substrates. - *Ibid.*, symp.A, p.A-19.
- A-162. Kotomin E.A. Atomistic theory of thin metal film growth on ionic substrates. - *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<sub>2</sub>O<sub>3</sub> (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<sub>3</sub> (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<sub>3</sub> 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<sub>3</sub> 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  $\text{KNbO}_3$  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  $\text{SrTiO}_3$ . – 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  $\text{ABO}_3$  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  $\text{SrTiO}_3$ . – Ibid., p. 31.

A-185. Heifets E., Eglitis R.I., Kotomin E.A. and Borstel G. *Ab initio* Calculations for  $\text{SrTiO}_3$  (100) Surface Structure. – Abstracts of Williamsburg Meeting on Fundamental 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  $\text{ABO}_3$  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  $\text{SrTiO}_3$  perovskite. — Ibid., p.43.

A-189. Heifets E., Evarestov R.A., Kotomin E.A., Dorfman S. Modelling of Polar (110) Oxygen-terminated Surface of  $\text{LaMnO}_3$  — Abstr. E-MRS Meeting, Strasburg, June 2003, Symp.N: New Materials and technologies in sensor applications, p. N20.

A-190. Zhukovskii 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  $\text{SrTiO}_3$  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  $\text{ABO}_3$  perovskites. — Ibid., p.121.

A-193. E.A. Kotomin, J. Maier, and E. Heifets. Hartree– Fock Calculations of the Surface Structure for  $\text{ABO}_3$  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  $\text{ABO}_3$  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  $\text{SrTiO}_3$ . – 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, Warszawa, 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  $\text{LaMnO}_3$ . – 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  $\text{BaSrTiO}_3$  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  $\text{SrTiO}_3$ ,  $\text{BaTiO}_3$  and  $\text{PbTiO}_3$  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  $\text{ABO}_3$  Perovskites and  $\text{MgO}$ . – 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  $\text{Cu/MgO}(100)$  interface. – Ibid., p.200.

A-204. Dorfman S., Piskunov S., Kotomin E.A., Fuks D. Calculations of the atomic and electronic structure of  $\text{BaSrTiO}_3$  (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 manganates. – 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  $\text{MgO}(001)$  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  $\text{AgCl}(111)$  surface and  $\text{AgCl}(111)/\alpha\text{-Al}_2\text{O}_3(0001)$  interface. – Ibid., Abstract H-P.26

A-209. Kotomin E.A. and Heifets E. First principles calculations of the atomic and electronic structure of  $\text{ABO}_3$  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  $\text{ABO}_3$  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  $\text{SrTiO}_3$  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  $\text{ABO}_3$  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  $\text{SrTiO}_3$  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  $\text{SrTiO}_3$  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  $\text{RuO}_2$  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  $\text{SrTiO}_3$ ,  $\text{PbTiO}_3$ ,  $\text{BaTiO}_3$  (001) and  $\text{BaTiO}_3$  (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  $(\text{La}_{7/8}\text{Sr}_{1/8})\text{MnO}_3$ , 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  $\text{SrFe}_x\text{Ti}_{1-x}\text{O}_{3-y}$ , Ibid., P-489.

A-222. Zhukovskii Yu.F., Kotomin E.A., and Ellis D. First principles simulation on the defect-free  $\text{Cu}/\text{BaTiO}_3(001)$  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 adsorption on perfect and defective  $\text{MgO}(001)$  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 adsorption on  $\text{MgO}$ . 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 adsorption on  $\text{MgO}$ . 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  $\text{AgCl}/\alpha\text{-Al}_2\text{O}_3$  (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 Zvejniaks 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-ameridium 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<sub>3</sub>(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<sub>3</sub> 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<sub>3</sub> 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., Zhukovskii 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  $\text{PbZrO}_3$  and  $\text{SrTiO}_3$  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  $\text{MgO}(001)$  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  $\text{MgO}(001)$  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 chemisorption on the  $\text{UN}(001)$  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  $\text{LiF}$  or  $\text{Li}_2\text{O}$ : 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  $\text{UN}(001)$  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  $\text{CaFeO}_3$  and  $\text{SrFeO}_3$ .



Ibid., Abstracts: p. 88.

A-256. S. Piskunov, E. Spohr, T. Jacob, E. Heifets, E.A. Kotomin, and D.E. Ellis. Thermodynamic stability of  $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$  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 Society (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  $\text{Li}_2\text{O}$ : experimental studies and theoretical simulations. Ibid. p.22.

A-260. Yu.F. Zhukovskii, E.A. Kotomin, S. Piskunov, and Yu.A. Mastrikov. The effect of oxygen vacancies on the atomic and electronic structure of cubic  $\text{ABO}_3$  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  $\text{ABO}_3$  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  $\text{SrTiO}_3$ . 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  $\text{UN}(001)$  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  $\text{ABO}_3$  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 LaMnO<sub>3</sub> and La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub> (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)MnO<sub>3</sub> 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 ABO<sub>3</sub> 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 CaF<sub>2</sub>: 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 nuclear 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 ABO<sub>3</sub> 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. Matrikov, R. Merkle and J. Maier, Oxygen incorporation reaction into mixed conducting ABO<sub>3</sub> - 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 ABO<sub>3</sub> 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 LaCoO<sub>3</sub>. *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 CaF<sub>2</sub>. *Ibid.*, p.185.
- A-293. R. I. Eglitis and E.A. Kotomin, Ab initio calculations of Nb-doped SrTiO<sub>3</sub>. *Ibid.* p. 186.
- A-294. R.I. Eglitis, A.F. Vassilyeva, E.A. Kotomin and A.K. Dauletbekova, Ab initio calculations of MgF<sub>2</sub> (001) and (011) surfaces. *Ibid.*, p. 187.
- A-295. E.A. Kotomin, Yu.A. Matrikov, M.M. Kuklja, R. Merkle, and J. Maier, First principles calculations of oxygen vacancy formation and migration in mixed conducting ABO<sub>3</sub>-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 SrTiO<sub>3</sub>. 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 PuO<sub>2</sub>. 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 SrTiO<sub>3</sub>. –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 MgF<sub>2</sub> (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 SrTiO<sub>3</sub> 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 MgF<sub>2</sub>. *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 PuO<sub>2</sub>. *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).

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. Mastrikov, M.M. Kuklja, and J. Maier, First principles modeling of oxygen vacancy formation and mobility in (Ba,Sr)(Co,Fe)O<sub>3</sub> 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)CoO<sub>3</sub> 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 PuO<sub>2</sub>. 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 SrTiO<sub>3</sub> 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)O<sub>3</sub> and SrTiO<sub>3</sub>. 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 SrTiO<sub>3</sub>. *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 CaF<sub>2</sub>. *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 MgF<sub>2</sub> crystals. *Ibid.*, Abstracts, p. 305.

A-345. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, and A. Mslang, 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 MgF<sub>2</sub> 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 mononitride. *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 La<sub>1-x</sub>Sr<sub>x</sub>Co<sub>1-y</sub>Fe<sub>y</sub>O<sub>3</sub> 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)O<sub>3</sub> 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 (La<sub>x</sub>Sr<sub>1-x</sub>)CoO<sub>3</sub>. *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. Mslang, 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 ABO<sub>3</sub> 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 MgF<sub>2</sub> 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 (La<sub>x</sub>,Sr<sub>1-x</sub>)CoO<sub>3</sub> 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 ABO<sub>3</sub>-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 ABO<sub>3</sub> 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<sub>x</sub>,Sr<sub>1-x</sub>)CoO<sub>3</sub>: 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 CaF<sub>2</sub> 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. Mslang, 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 CaF<sub>2</sub>. *Ibid.*, Abstract: PO-30.

A-372. F.U. Abuova, A.T. Akilbekov, E.A. Akilbekov, and S. Piskunov, First-principles calculations of defects in MgF<sub>2</sub>. *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<sub>3</sub> 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<sub>3</sub> perovskites based on ab initio modeling. – Bunsentagung 2013 meeting [Annual meeting of German Physical Chemistry Society] (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 fuel 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.