CURRICULUM VITAE OF Dr. ROBERTS I. EGLITIS

Family name: Eglitis
First name: Roberts
Date of birth: February 1, 1966
Present address: Department of Physics and Astronomy
Rutgers University
136 Frelinghuysen Road, Piscataway, NJ 08854-8019, USA
e-mail: reglitis@physics.rutgers.edu; phone: +1-732-445-4197

AWARDS

Year: 1984 - Second place in the physics competitions between secondary schools of all Baltic Countries

EDUCATION

1984 IX - 1991 VI Student at the University of Latvia. Academic degrees: B.S.+M.S.
1984 X -1986 XI Break of studies for military service.
1991 XI - 1994 VI PhD student at the Institute of Solid State Physics, University of Latvia.
Academic degree: 1994 VI, Dr. of Physics (PhD)
Title of Thesis: Theoretical modeling of radiation-induced Frenkel defects correlated annealing kinetics in $AgBr_{1-x}Cl_x$, KBr and KCl crystals. Supervisor: Prof. Dr. E.A. Kotomin

ACADEMIC AND PROFESSIONAL EXPERIENCE

1984-1991 Student of the Latvian University + Engineer at the Inst. of Solid State Phys., Univ. of Latvia
1988-1995 Engineer at the Institute of Solid State Physics, University of Latvia
1995 – today Researcher and Leading Researcher at Inst. of Solid State Physics, Univ. of Latvia
1994 IX-1995 IX Postdoctoral Position at Department of Physics, Linköping University, Sweden
1995 X –1998 VII Postdoctoral Position at Department of Physics, Osnabrück University, Germany
1998 VII-1999 XII Visiting Research Fellow, Institute of Materials Research and Engineering, Singapore
2000 IV – IV 2006 Resarch Assistant at the Osnabrück University, Germany (C1 position)
2006 X – 2007 V Researcher Associate, Sung Kyun Kwan University, Suwon, South Korea
2007 VIII – today Visiting Research Fellow, Department of Physics and Astronomy, Rutgers University, USA

GRANTS:

1) Volkswagen-Foundation Grant for the young scientists (01.04.1998. – 31.03.2000.).
2) NATO collaborative grant on Defects in perovskites (2001 – 2003).
3) German Research Council Grant for the hiring of the PhD student (DFG grant EG 133/2-1) (01.02.2001. – 31.01.2004.).
4) NATO Linkage grant on perovskite surfaces and defects (2004 – 2006).
5) Accionas Integradas, Cooperation grant with Spain (DAAD) (1.1.2004. – 1.1.2006.)
6) Research stipendium for 12 months work at Professor D. Vanderbilt group, Rutgers University, USA (01.08.2007.-31.07.2008). (DFG; GZ: EG 133/11-1; AOBJ: 538704).

MEMBER OF THE:

American Materials Research Society 2001-2003
Singapore Materials Research Society 2003-June 30, 2007

STUDENTS:

Co-supervisor of a PhD student S. Piskunov, DFG project EG 133/2-1 (01.02.2001. – 31.01.2004.).
Co-Supervisor of a PhD student Shi Hong-Ting (01.03.2004. – 28.02.2007.).
Co-Supervisor of the Diploma student M. Kadiroglu (01.01.2004. – 01.01.2005.).
Supervisor of the Master student A. Gopejenko (01.10.2006 - 05.06.2007).

TEACHING at the Osnabruck University, Germany:

1) Winter Semester: October 1, 2000 – February 13, 2001, Mechanics + Elektrodynamics (Exercises).
2) Summer Semester: April 1, 2001 - July 13, 2001, Quantum Mechanics + Thermodynamics, (Exercises).
3) Winter Semester: Oktober 1, 2001 – February 13, 2002, Mechanics + Electrodynamics, (Exercises).
4) Summer Semester: April 1, 2002 – July 13, 2002, Extension of Theoretical Physics II (Quantum Mechanics + Thermodynamics, Exercises).
5) Winter Semester: October 1, 2002 – February 13, 2003. Regular lectures: Methods of Mathematical Physics (for more as 30 students).
   Exercises in Methods of Mathematical Physics.
6) Summer Semester: April 1, 2003 – July 13, 2003. Methods of Mathematical Physics (Exercises).
   Lectures: Computational Methods in Materials Science, Part I.
7) Winter Semester: Oktober 1, 2003 – Februar 7, 2004,
   Lectures: Computational Methods in Materials Science, Part II.
   Exercises: Methods of Mathematical Physics
   Exercises: Numerical Methods in Physics
8) Summer Semester: April 1, 2004 – July 13, 2004.
   Lectures: Computer Modeling of Materials at Atomic Level.
   Exercises. Introduction into Theoretical Physics II (Quantum Mechanics + Thermodynamics).
9) Winter Semester: October 1, 2004 - February 13,2005.
   Lectures: *Ab initio* Methods in Materials Science, Part I.
   Exercises: Introduction into Theoretical Physic I (Mechanics + Electrodynamics) (attended 45 students).
10) Summer Semester: April 1, 2005 – July 13, 2005.Excersises: Extension of Theoretical Physics II (Quatum Mechanics + Thermodynamics). Lectures: *Ab initio* Methods in Materials Science, Part II.
11) Winter semester: October 1, 2005 – February 13, 2006.
    Exercises: Extension of Theoretical Physics I (Mechanics + Elektrodynamics).
    Lectures: Computer modelling in Materials Science.

PUBLICATIONS: I am author and co-author of **112** papers in refereed journals and **116** Conference Abstracts. My h-index is **14**.

The 12 most cited papers according to the Web of Science are:

1. E. Heifets, R.I. Eglitis, E.A. Kotomin, J. Maier, and G. Borstel, Phys. Rev. B **64**, 235417, 2001. Cited **71** times.
2. R.I. Eglitis, A.V. Postnikov, and G. Borstel, Phys. Rev. B 54, 2421, 1996. Cited **52** times.
3. R.I. Eglitis, A.V. Postnikov, and G. Borstel, Phys. Rev. B **55,** 12976, 1997. Cited **48** times.

4. R.I. Eglitis, N.E. Christensen, E.A. Kotomin, A.V. Postnikov, and G. Borstel, Phys. Rev. B **56,** 8599, 1997. Cited **46** times.
5. E. Heifets, R.I. Eglitis, E.A. Kotomin, J. Maier, and G. Borstel, Surface Science **513**, 211, 2002. Cited **39** times.
6. E.A. Kotomin, R.I. Eglitis, A.V. Postnikov, G. Borstel, and N.E. Christensen, Phys. Rev. B **60,** 1, 1999. Cited **29** times.
7. E.A. Kotomin, M.M. Kuklja, R.I. Eglitis, and A.I. Popov, Materials Science and Engineering B **37,** 212, 1996. Cited **28** times.
8. S. Piskunov, E. Heifets, R.I. Eglitis, and G. Borstel, Comput. Mat. Sci. **29**, 165, 2004. Cited **38** times.
9. V.S. Vikhnin, R.I. Eglitis, S.E. Kapphan, E.A. Kotomin, and G. Borstel, Europhysics Letters **56**, 702, 2001. Cited **26** times.
10. E.A. Kotomin, R.I. Eglitis, and G. Borstel, J. Phys. Cond. Matter **12,** L557, 2000. Cited **26** times.
11. E.A. Kotomin, R.I. Eglitis, and A.I. Popov, J. Phys. Cond. Matter **9**, L315, 1997. Cited **25** times.
12. S. Piskunov, E.A. Kotomin, E. Heifets, J. Maier, R.I. Eglitis, and G. Borstel, Surface Science **575**, 75 (2005). Cited **25** times.

INVITED TALKS: I had a number of invited talks at the International Conferences, including 4 invited talks at USA:

1. R.I.Eglitis, E.A.Kotomin, A.V.Postnikov, N.E.Christensen, G.Borstel, First-principles and semiempirical Hartree-Fock calculations for *F* centers in $KNbO_3$ and Li impurities in $KTaO_3$,- Fifth Williamsburg Workshop on First-Principles Calculations for Ferroelectrics, February 1-4, Colonial Williamsburg, USA, p. 22, 1998 (**Invited Talk**).
2. R.I. Eglitis, M.R. Philpott and S.V. Izvekov, Computer modelling of corrosion, 2001 MRS Spring Meeting, April 16-20, 2001, SanFrancisco, California, USA, p. 331. (**Invited Talk**).
3. R.I. Eglitis, E.A. Kotomin, G. Borstel, and V.S. Vikhnin, Quantum chemical modeling of polarons and excitons in ABO_3 perovskites, Fundamental Physics of Ferroelectrics, February 2-5, 2003, Williamsburg, Virginia, USA, Abstract book, pp. 43. (**Invited Talk**).
4. R.I. Eglitis, and J. Lee, *Ab initio* calculations of perovskite surfaces, Fundamental Physics of Ferroelectrics, Colonial Williamsburg, VA, February 11-14, 2007, Abstract book, pp. 35-36. (**Invited Talk**).

LANGUAGES: English, German, Latvian, Russian.

MAIN SCIENTIFIC INTERESTS

During my MS study, my scientific interests have been connected with large-scale computer simulations of the kinetics of the primary radiation defect recombination in ionic solids (KBr, KCl and mixed $AgBr_{1-x}Cl_x$ crystals). On graduating from the University in 1991, I continued this direction of research during my PhD studies and I have defended my PhD thesis "Theoretical modeling of radiation-induced Frenkel defects correlated annealing kinetics in $AgBr_{1-x}Cl_x$, KBr, KCl crystals" in 1994, under supervision of Prof. Dr. E.A. Kotomin. During this research, I developed a theory of diffusion-controlled recombination of two kinds of primary Frenkel defects in alkali halide crystals - pairs of neutral defects (called *F*,*H* centers) and oppositely-charged (α, *I*) defects. In a kinetic model we took into account defect diffusion and the elastic/Coulomb interactions between *F*,*I* and α,*I* partners, respectively. We demonstrated that the tunneling recombination play an essential role at low temperatures. All calculations have been done using a code written by me.

After PhD studies, I switched my scientifical interests to the large-scale quantum chemical simulations of static and dynamic properties of defects in ionic solids/semiconductors based on the semi-empirical quantum chemical method of the Intermediate Neglect of Differential Overlap (INDO). Such theoretical approach allowed us to study big quantum clusters (about 200-300 atoms) in technologically important ceramic materials (MgO and Al_2O_3), complex defects (like dimer F_2 -centers), to optimize the defect geometry, as well as to model theoretically the defect diffusion barriers, which is important for a better understanding of many reactions in solids, including the process of colloid formation in oxides.

During the last years, I have focused my scientifical interests on ferroelectric perovskites. We applied the INDO method to ferroelectric materials, which allowed us to treat considerably larger supercells, (up to 270 atoms in the case of Li doped $KTaO_3$) which, taking into account the enormous computational efforts, is prohibited for a first-principles approach. We have demonstrated that the accuracy of the INDO method is sufficient for adequately describing the small energy differences related to the ferroelectric instability in $KNbO_3$. The choice of INDO parameters has been done for the first time for a system containing Nb and Ta. Based on the parametrization proposed, the electronic structure, equilibrium ground state structure of the orthorhombic and rhombohedral phases, and Γ-TO phonon frequencies in cubic and rhombohedral phases of $KNbO_3$ were calculated and found to be in good agreement with the experimental data and first principle calculations available. The INDO method also gave very good results for non-ferroelectric $KTaO_3$. Total-energy results for $KTaO_3$ as pure crystal (concentrating on frozen phonon calculations) and that with Li impurities have been found in good agreement with the available experimental data and first principle calculations. We have also used the INDO + LMTO method for a study of defects (hole polarons + *F* centers) in perovskite-based ferroelectric $KNbO_3$ crystals. We demonstrated that the *F* center in $KNbO_3$ reminds much more electron defects in a partly-covalent SiO_2 crystal, rather than usual *F* centers in ionic crystals like MgO and alkali halides.

My current scientifical activities are partly connected with *ab initio* studies of ferroelectric material surfaces. For example, we performed *ab initio* calculations of $SrTiO_3$ (100) surface relaxation and rumpling with two different terminations (SrO and TiO_2). These are based on *ab initio* Hartree-Fock method with electron correlation corrections and density functional theory calculations with different exchange-correlation functionals, including hybrid exchange techniques. All methods agree well on surface energies and on atomic displacements, as well as on considerable increase of covalency effects nearby the surface.

Recently we demonstrated, that the best agreement with experiment for the CaF_2 optical band gap (12.1 eV) can be obtained using a hybrid Hartree-Fock and density-functional theory exchange functionals, using Beckes three-parameter method, combined with the nonlocal correlation functionals by Perdew and Wang (10.96 eV). We also presented calculations of CaF_2 (111), (110), and (100) surfaces. Our calculated surface energies confirm that the CaF_2 (111) surface is the most stable one, in agreement with the experiment. The characterization of *F* centers in CaF_2 is still a question of debate. In order to understand the behaviour of the material with respect to its optical properties, we performed *ab initio* calculations to determine the electronic structure, atomic geometry, and formation energy of *F* center in CaF_2.

Currently the lithium-ion batteries are the state of the art power sources for consumers electronics operating mainly in the 4 V regime. One frequently discussed direction to improve the performance of such batteries is the development of 5 V cathode materials. Based on the results of our *ab initio* calculations we first in the world predicted the existence of 5 V battery.

Dr. R.I. EGLITIS SCIENTIFIC PAPERS IN REFEREED JOURNALS

1. D. Millers, L. Grigorjeva, E. Kotomin, E. Krivads, and **R.I. Eglitis**, High excitation density luminescence as probe of mixed silver halides, - Proc. SPIE (Infrared Fiber Optics 3), **1591**, pp. 157-165, 1992.
2. E.A. Kotomin, **R.I. Eglitis**, and A.I. Popov, Kinetics of correlated annealing of radiation defects in ionic solids, - Nucl. Instr. & Meth. in Phys. Res. B, **65**, p.512-515, 1992.
3. E.A. Kotomin, A.I. Popov, and **R.I. Eglitis**, Correlated annealing of radiation defects in KBr crystals, - J. Phys. Cond. Matter, 1992, **4**, p. 5901-5910, 1992.
4. E.A. Kotomin, **R.I. Eglitis**, and A.I.Popov, Kinetics of correlated diffusion-controlled annealing of Frenkel defects in alkali halide crystals, - In: Proceedings of the 12 Int. Conf. on Defects in Insulating Materials (World Scientific, Singapore, 1992), **2**, p. 1004-1006, 1992.
5. D.K. Millers, L.G. Grigorjeva, E.A. Kotomin, and **R.I. Eglitis**, Intrinsic luminescence of mixed silver halides under powerful excitation as a probe of solid solution composition,- In: Proceedings of the 12th Int. Conf. on Defects in Insulating Materials (World Scientific, Singapore, 1992), **2**, p. 1277-1280, 1992.
6. E.A. Kotomin, A.I. Popov, and **R.I. Eglitis**, The kinetics of correlated annealing of *F*,*I* centres in KBr crystals,- Phys. Stat. Solidi (b), **175**, K39-42, 1993.
7. L.G. Grigorjeva, D.K. Millers, E.A. Kotomin, **R.I. Eglitis**, Short-lived luminescence of mixed silver halides,- J. of Luminescence, **55**, p. 243-252, 1993.
8. E.A. Kotomin, **R.I. Eglitis**, and A.I. Popov, The kinetics of diffusion - controlled annealing of Frenkel defects in alkali halide crystals,- Nucl. Instr. & Meth. in Phys. Res. B **91**, p. 83-86, 1994.
9. E. Kotomin, D. Millers, L.Grigorjeva, and **R.Eglitis**, The kinetics of excitonic luminescence in mixed silver halides,- Proceedings of MRS Spring Meeting, Symposium P, San-Francisko, p. 309-312, 1994.
10. L.G. Grigorjeva, E.A.Kotomin, D.K.Millers, and **R.I.Eglitis**, The decay kinetics of excitonic luminescence in AgCl crystals, - J.Phys. Cond. Matter **7**, p. 1483-1491, 1995.
11. **R.I.Eglitis**, A.I.Popov, and E.A.Kotomin, Computer Simulations of *I*-center Annealing in KCl and KBr Crystals: Theoretical Interpretation of Thermostimulated Experiments, - Phys. Stat. Solidi (b) **190**, p. 353, 1995.
12. A.I.Popov, E.A.Kotomin, and **R.I.Eglitis**, Theoretical Simulations of *I*-Center Annealing in KCl Crystals,- Radiation Effects & Defects in Solids, **134**, p. 83 - 86, 1995.
13. L.G. Grigorjeva, D.K. Millers, E.A. Kotomin, **R.I. Eglitis**, L.I. Lerman, Optical properties of Silver Halide Fibers: Extrusion and Aging Effects, - J. Phys. D: Appl. Phys., **29**, p. 578 - 583, 1996.
14. E.A.Kotomin, M.M.Kuklja, **R.I.Eglitis**, and A.I.Popov, Quantum Chemical Simulations of the Optical Properties and Diffusion of Electron Centers in MgO Crystals, - Materials Science & Engineering B **37**, p. 212-214, 1996.
15. **R.I.Eglitis**, M.M.Kuklja, E.A.Kotomin, A.Stashans, and A.I.Popov, Semi - empirical simulations of the electron centers in MgO crystal, - Computational Materials Science, **5**, p. 298-306, 1996.
16. **R.I.Eglitis**, A.V.Postnikov, and G.Borstel, Semiempirical Hartree - Fock calculations for $KNbO_3$, - Phys. Rev. B, **54**, p. 2421 - 2427, 1996.
17. **R.I.Eglitis**, A.V.Postnikov, and G.Borstel, Semiempirical Hartree - Fock calculations for $KNbO_3$ and $KTaO_3$,- Proc. SPIE (Proc. of AOMD - 96 Conf., Riga, 1996), **2967**, p.144-149, 1997.
18. **R.I.Eglitis**, A.V.Postnikov, and G.Borstel, Semiempirical Hartree - Fock calculations for pure and Li

– doped $KTaO_3$, - Phys. Rev. B, **55**, p. 12976 - 12981, 1997.

19. **R.I.Eglitis**, N.E.Christensen, E.A.Kotomin, A.V.Postnikov, and G.Borstel, First-principles and semi-empirical calculations for *F* centers in $KNbO_3$ crystal, - Phys. Rev. B, **56**, p. 8599 - 8604, 1997.
20. E.A.Kotomin, **R.I.Eglitis**, and A.I.Popov, Charge distribution and optical properties of F^+ and *F* centers in $KNbO_3$ crystal, - J. Phys. Cond. Matter, **9**, L315-L321, 1997.
21. **R.I.Eglitis**, and E.A.Kotomin, Calculations of *F* centers in $KNbO_3$ ferroelectric crystals, - Proc. SPIE (Proc. of AOMD-96 Conf., Riga, 1996), **2967**, p.150-152, 1997.
22. E.A.Kotomin, N.E.Christensen, **R.I.Eglitis**, and G. Borstel, A comparative study of the atomic and electronic structure of *F* centers in ferroelectric $KNbO_3$: *ab initio* and semi-empirical calculations, - Computational Materials Science **10**, pp. 339-345, 1998.
23. **R.I.Eglitis**, E.A.Kotomin, A.V.Postnikov, N.E.Christensen, and G.Borstel, First-principles and semi-empirical Hartree-Fock calculations for *F* centers in $KNbO_3$ and Li impurities in $KTaO_3$, - Proc. AIP (Proceedings of 5th Williamsburg Meeting of Ferroelectric Materials, Williamsburg, USA, 1998), **436**, pp. 207- , 1998.
24. **R.I.Eglitis**, V.S.Vikhnin, P.A.Markovin, G.Borstel, Self-ordered second-component clusters in solid solutions on the basis of ferroelectric perovskites: Nb clusters in $KTaO_3$,- Proc. AIP (Proceedings of 5th Williamsburg Meeting of Ferroelectric Materials, Williamsburg, USA, 1998), **436**, pp. 87- , 1998.
25. **R.I.Eglitis**, E.A.Kotomin, and G.Borstel, Semi-Empirical Calculations of Hole Polarons in MgO and $KNbO_3$ Crystals,- Phys. Status Solidi (b), **208**, 15-20, 1998.
26. **R.I.Eglitis**, E.A.Kotomin, G.Borstel, S. Dorfman, Semi-empirical calculations of the Nb-ion positions in doped $KTaO_3$ crystals, - J. Phys. Condens. Matter **10**, 6271-6276, 1998.
27. **R.I.Eglitis**, A.V. Postnikov, G.Borstel, Semiempirical Hartree-Fock simulations of lattice relaxation and effective interactions in Li-doped $KTaO_3$,- Phys. Status Solidi (b), **209**, 187-193, 1998.
28. **R.I. Eglitis**, E.A. Kotomin, and G. Borstel, Quantum chemical calculations of KTN solid solutions, - Solid State Communications, **108**, pp. 333-336, 1998.
29. **R.I. Eglitis** and E.A. Kotomin, Calculations of hole polaron properties in oxide crystals, Computer Modeling & New Technologies **2**, pp. 21-24, 1998.
30. V.S.Vikhnin, **R.I.Eglitis**, P.A.Markovin, G.Borstel, Self - ordered second-component Nb clusters in $KNb_xTa_{1-x}O_3$ solid solution and their physical properties,- Phys. Status Solidi (b), **212**, pp. 53-63, 1999.
31. V.S. Vikhnin, **R.I. Eglitis**, P.A. Markovin, G. Borstel, Self-ordered clusters of second-component in solid solutions on the basis of ferroelectric perovskites: Nb clusters and single Nb ion in $KTaO_3$, Inorganic Materials, **35**, pp. 823-827, 1999.
32. P.W.Jacobs, E.A.Kotomin, and **R.I.Eglitis**, Semi-empirical INDO and shell-model calculations for perovskites, Radiation Effects & Defects in Solids, **151**, pp. 243-247, 1999.
33. **R.I.Eglitis**, E.A.Kotomin, A.V.Postnikov, N.E.Christensen, M.A. Korotin, G.Borstel, Computer simulations of defects in perovskite $KNbO_3$ crystals, Ferroelectrics, **229**, pp. 69-75, 1999.
34. **R.I.Eglitis**, A.V.Postnikov, G.Borstel, Semiempirical Hartree – Fock calculations for single and interacting Li impurities in $KTaO_3$, Ferroelectrics, **229**, pp. 63-67, 1999.
35. E.A. Kotomin, **R.I. Eglitis**, A.V. Postnikov, G. Borstel, and N.E. Christensen, First - principles and semi-empirical calculations for bound hole polarons in $KNbO_3$, Phys. Rev. B, **60**, pp. 1-5, 1999.
36. V.S. Vikhnin, H. Liu, W. Jin, S. Kapphan, **R.I. Eglitis**, and D. Usvyat, Critical effects in optical response due to charge transfer vibronic excitons and their structure in perovskite-like systems,

Journal of Luminescence, **83-84**, pp. 109-113, 1999.

37. S. Izvekov, M.R. Philpott, and **R.I. Eglitis**, *Ab Initio* Simulation of Metal Cluster Surrounded by Electrolyte, Journal of The Electrochemical Society **147**, pp. 2273-2278, 2000.
38. **R.I. Eglitis**, S.V. Izvekov, and M.R. Philpott, Metal Dissolution in Aqueous Electrolyte. Semi-empirical Hartree-Fock and *ab initio* MD Calculations, Computational Materials Science **17**, pp. 275-278, 2000.
39. P.W. M. Jacobs, E.A. Kotomin, and **R.I. Eglitis**, Semi-empirical defect calculations for the perovskite $KNbO_3$, J. Phys.: Condens. Matter **12**, pp. 569-574, 2000.
40. E.A. Kotomin, **R.I. Eglitis**, G. Borstel, Quantum Chemical Modelling of point defects in $KNbO_3$ perovskite crystals, Computational Materials Science **17**, pp. 290-298, 2000.
41. N.E. Christensen, E.A. Kotomin, **R.I. Eglitis**, A.V. Postnikov, G. Borstel, D.L. Novikov, S.Tinte, M.G. Stachiotti, and C.O. Rodriguez, Quantum mechanical modelling of pure and defective $KNbO_3$ perovskites, In: Defects and Surface-Induced Effects in Advanced Perovskites, ed. G. Borstel, NATO Science Series, High Technology, **77**, pp. 3-16, 2000.
42. A.V. Postnikov, G. Borstel, A.I. Poteryaev, and **R.I. Eglitis**, First - principles simulations of substitutional defects in perovskites, In: Defects and Surface-Induced Effects in Advanced Perovskites, ed. G. Borstel, NATO Science Series, High Technology, **77**, pp. 17-26, 2000.
43. E.A. Kotomin, **R.I. Eglitis**, G. Borstel, L.G. Grigorjeva, D.K. Millers, and V. Pankratov, Theoretical and experimental study of radiation defects in $KNbO_3$ perovskite crystals, Nuclear Instruments and Methods in Physics Research B, **166-167**, pp. 299-304, 2000.
44. A.V. Postnikov, **R.I. Eglitis**, V. Caciuc, and G. Borstel, First-Principles Simulations of Ferroelectric Oxides, Ferroelectrics, **236**, pp. 47-58, 2000.
45. **R.I. Eglitis**, E.A. Kotomin, and G. Borstel, Quantum chemical modelling of perovskite solid solutions, J. Phys.: Condens. Matter **12**, L431-L434, 2000.
46. E.A. Kotomin, **R.I. Eglitis**, and G. Borstel, Quantum chemical modelling of electron polarons and excitons in ABO_3 perovskites, J. Phys.: Condens. Matter **12**, L557-L562, 2000.
47. G. Borstel, E.A. Kotomin, **R.I. Eglitis** and E. Heifets, Computer modelling of point defects, impurity self-ordering effects and surfaces in advanced perovskite ferroelectrics, Acta Physica Polonica A **98**, pp. 469-481, 2000.
48. G. Borstel, E.A. Kotomin, **R.I. Eglitis** and E. Heifets, Computer modeling of defects and surfaces in advanced perovskite ferroelectrics, Jpn. J. Appl. Phys. Vol. **39**, S**39-1**, 24-28, 2000.
49. G. Borstel, **R.I. Eglitis**, and E.A. Kotomin, Computer modelling of KTN solid solutions, In: Proceedings of the 2000 12th IEEE International Symposium on Applications of Ferroelectrics, (edited by S.K. Streiffer, B.J. Gibbons, and T.Tsurami), *The Institute of Electrical and Electronics Engineers Ultrasonics, Ferroelectrics, and Frequency Control Society* (IEEE Catalog Number 00CH37076) **2**, 671-674, 2001.
50. J.T. Devreese, V.M. Fomin, E.P. Pokatilov, E.A. Kotomin, **R.I. Eglitis**, and Yu.F. Zhukovskii, Theory of bound polarons in oxide compounds, Phys. Rev. B **63**, 184304, 2001.
51. V.S. Vikhnin, **R.I. Eglitis**, E.A. Kotomin, S. Kapphan and G. Borstel, New Polaronic-Type Excitons in Ferroelectric Oxides: INDO-Calculations and Experimental Manifestation, Mat. Res. Soc. Symp. Proc. Vol. **677**, AA4.15.1-AA4.15.6, 2001.
52. **R.I. Eglitis**, E.A. Kotomin and G. Borstel, Quantum Chemical Modelling of Polarons and Perovskite Solid Solutions, Computational Materials Science **21**, 530-534, 2001.

53. E. Heifets, **R.I. Eglitis**, E.A. Kotomin, J. Maier and G. Borstel, *Ab initio* modelling of surface structure for $SrTiO_3$ perovskite crystals, Physical Review B **64**, 235417, 2001.
54. **R.I. Eglitis**, E.A. Kotomin and G. Borstel, Computer Modeling of Luminescence in ABO_3 Perovskites, Mat. Res. Soc. Symp. Proc. Vol. **667**, G1.8.1.-G1.8.6, 2001.
55. E.Heifets, **R.I. Eglitis**, E.A. Kotomin, and G. Borstel, First - principles and Semi - Empirical Calculations of Atomic and Electronic Structure for (100) and (110) Perovskite Surfaces, in Fundamental Physics of Ferroelectrics 2001, edited by H. Krakauer, AIP Conference Proceedings Vol. **582**, p. 201, AIP, New York, 2001.
56. V.S. Vikhnin, **R.I. Eglitis**, E.A. Kotomin, S. Kapphan and G. Borstel, New-Polaronic Type Excitons in Ferroelectric Oxides: Nature and Experimental Manifestation, in Fundamental Physics of Ferroelectrics 2001, edited by H. Krakauer, AIP Conference Proceedings Vol. **582**, p. 228, AIP, New York, 2001.
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