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AUTOREFERAT

1. Personal data

Mikhail G. Brik
born on January 30, 1969, Krasnodar region, Russia
Home address: A. Vabbe 6 - 5, Tartu 51011, Estonia

2. Present working place:

Institute of Physics, University of Tartu,
Riia 142, Tartu 51014, Estonia
Professor of Computational Materials Science

3. Scientific degrees and titles

Post-graduate: 2001 – Docent certificate (Ministry of Education of the Russian Federation)

1995 – PhD (candidate of physical and mathematical sciences),
Kuban State University, Krasnodar, Russia.

Specialization: solid state physics, the title of dissertation *Non-radiative transitions in impurity centers with strong electron-vibrational interaction*,
Advisor: Prof. Dr. Sci. V.F. Pisarenko

Graduate: 1992 – MSc in physics, physical faculty, Kuban State University, Krasnodar, Russia.
Specialization: Physics; Qualification obtained: engineer-physicist.
The diploma project: *Spectra of Cr^{4+} ions in Y_2SiO_5 and $Y_3Al_5O_{12}$ crystals*
Advisors: Associate Professor Dr. A.G. Avanesov, V.V. Zhorin,
– ***diploma with distinction,***
– ***First Degree diploma, USSR Students' conference on physical optics, Tomsk, May 1991***

School 1975 - 1985 – School No. 48, Chernoerkovskaya, Slavyanskii raion, Krasnodarskii krai. Gold medal awarded.

4. Job history

February 2009 – present:	Professor of Computational Materials Science, Laboratory of Laser Spectroscopy, Institute of Physics, University of Tartu, Estonia
July 2008 – February 2009:	Extraordinary Senior Researcher, Laboratory of Laser Spectroscopy, Institute of Physics, University of Tartu, Estonia
July 2007 – July 2008:	Guest Professor, Laboratory of Laser Spectroscopy, Institute of Physics, University of Tartu, Estonia
March 2003 – July 2007	Visiting Researcher, Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto, Japan
July 2005 – November 2007	Visiting Researcher, Department of Chemistry, Kwansei Gakuin University, Sanda, Japan

December 2001 – December 2002	Visiting Researcher, Department of Chemical Physics, Weizmann Institute of Science, Rehovot, Israel
October 2000 – December 2001	Associate Professor, Department of Physics, University of Asmara, Asmara, Eritrea
March 1998 – October 2002	Associate Professor, General Physics Department, Kuban State University, Krasnodar, Russia
September 1997 – March 1998	Senior Lecturer, General Physics Department, Kuban State University, Krasnodar, Russia
May 1996 – September 1997	Junior Researcher, Experimental Physics Department, Kuban State University, Krasnodar, Russia
September 1992 – November 1995	Post-graduate, Experimental Physics Department, Kuban State University, Krasnodar, Russia
September 1985 – June 1992	Student, Physical faculty, Kuban State University, Krasnodar, Russia (including two years of a compulsory military service from June 1987 till June 1989)

5. Information about scientific publications

5.1. Total number of research articles = **190** (168 are listed in the Web of Science database), out of them 189 published after getting PhD degree. Total number of book chapters - **8** (all of them published after getting PhD degree). The articles were published in prestigious international journals, such as:

- **Journal of Physics: Condensed Matter** – 11 papers;
- **Physical Rewiev B** – 3 papers;
- **Inorganic Chemistry** – 2 papers;
- **Journal of American Chemical Society** – 1 paper;
- **Journal of Applied Physics** – 3 papers;
- **Journal of Physics D: Applied Physics** – 5 papers;

5.2. Total impact factor of published papers (according to the Journal Citation Reports database and web-pages of the corresponding journals; the data were taken for the publication year of each article): 255.696

5.3. Number of citaions of the above mentioned papers (Web of Science, 21.02.2012) = **823.**

Hirsch index = **15**.

5.4. Other creational professional work:

- 115 presentations at various international conferences, among them:
  a) 20 oral presentations (two of them invited), 19 presentations after getting PhD
  b) 95 poster presentations, among them 91 presentations after getting PhD,
- 14 invited seminars at diffrent research institutions and universities; all of them were organized after getting PhD.
- 5 manuals for students (two were published in Russian and three in English):
  - M.G. Brik, I.D. Bregeda, M.P. Matveyakin, "Methods of treatments of experimental results in physical laboratory" (in Russian), Krasnodar, Kuban State University, 1997. 73 pages.
  - M.G. Brik, I.D. Bregeda, M.P. Matveyakin, "Mechanics: problems with solutions" (in Russian), Krasnodar, Kuban State University, 2000. 112 pages.
  - M.G. Brik, S.S. Kotelnikov, M.Kahsay, "Physics 206: Electricity and Optics. Laboratory Manual", University of Asmara, Asmara, 2001. 56 pages.
  - M.G. Brik, S.S. Kotelnikov, "Kinematics: problems with solutions", University of Asmara, Asmara, 2001. 26 pages.
  - M.G. Brik, I. Sildos, V. Kiisk, "Introduction to spectroscopy of atoms, molecules and crystals", Tartu University Press, 2008, 234 pages.

6. Participation in the local and international research projects

6.A. Before getting PhD degree

No data available

6.B. After getting PhD

1999 – 2000: participant in a project of the Russian Foundation for Basic Research;

2003 - 2005: participant in the project funded by the Japanese Ministry of Education, Culture, Sports, Science and Technology (MEXT) „Computational Materials Science Unit at Kyoto University"

2007 - 2010: participant in the project funded by the Estonian Sceince Foundation „Stimulation and control of optical processes in oxide nanomaterials: applications in photonics and sensorics", finished 31.12.2010;

2007 - 2012: participant in the project funded by the Estonian Sceince Foundation „Low-dimensional structures and their applications", finished 31.12.2012;

2008 – 2010: participant in the project funded by the Estonian Sceince Foundation „Functionalization of rare earth activated metal-oxides for application as phosphors and sensors", finished 31.12.2010;

2010 – 2013: supervisor of the the project funded by the Estonian Sceince Foundation „Ab initio and semi-empirical modeling of optical properties of materials doped with rare-earth and transition metal ions", will be finished 31.08.2013;

2011 – 2013: participant in the the project funded by the Estonian Sceince Foundation „Temperature- and light-controlled defectiveness of metal oxides for application in optical gas sensing", will be finished 31.12.2013;

2011 – 2015: participant in the the project funded by the Estonian Sceince Foundation „Design of advanced nanostructured materials with tailored properties for novel laser and light sources", will be finished 31.07.2015;

7. List of the conferences, where the oral presentations were given (after getting PhD degree)

1. M.G. Brik, V.V. Zhorin, "Energy levels and non-radiative transitions probabilities calculations for Cr^{4+} in YAG", Int. Conf. on Luminescence and Optical Spectroscopy of Condensed Matter. Conf. Handbook, Prague, 1996. P.O2-8.
2. T. Ishii, K. Ogasawara, M.G. Brik, I. Tanaka, H. Ikeno, "First principles calculations of optical spectra of rare earth ions in laser crystals", Abstracts 2 Symposia: Category C &

D, The 8th International Conference on Advanced Materials, IUMRS–ICAM 2003, October 8-13, 2003, Yokohama, Japan. P. 280.

3. M.G. Brik, I. Tanaka, T. Ishii, "Lattice vibrations and their influence on impurity ion energy levels in laser crystals", Abstracts 2 Symposia: Category C & D, The 8th International Conference on Advanced Materials, IUMRS–ICAM 2003, October 8-13, 2003, Yokohama, Japan. P. 288.
4. T. Ishii, K. Ogasawara, S. Watanabe, I. Tanaka, H. Ikeno, M.G. Brik, "Calculations of rare-earth ions optical characteristics in a free state and crystals", Collected Abstracts of the 2003 Autumn Meeting of the Japan Institute of Metals, October 11-13, 2003. Sapporo, Japan. P. 264.
5. K. Ogasawara, S. Watanabe, H. Toyoshima, T. Ishii, M.G. Brik, H. Ikeno, I. Tanaka, "Optical spectra of trivalent lanthanides in $LiYF_4$ crystal", 227th Meeting of American Chemical Society, Anaheim, March 28–April 1, 2004, Paper NUCL 84 (also in the Abstracts of papers of the American Chemical Society 227: U88-U88 84-NUCL Part 2, MAR 28 2004).
6. T. Ishii, K. Ogasawara, M.G. Brik, "First principles calculations of spectral properties of luminescent materials doped with rare-earth ions", Extended abstracts of the 65th Autumn Meeting of the Japan Society of Applied Physics, Sendai, Japan, September 1-4, 2004, No. 3, p. 1264.
7. K. Ogasawara, S. Watanabe, H. Toyoshima, M. G. Brik, I. Tanaka, T. Ishii, "Nonempirical relativistic configuration-interaction calculation of $4f^n$ and $4f^{n-1}5d^1$ multiplet structures of trivalent lanthanides in YVO_4 crystal", Abstracts of the XII Feofilov symposium on spectroscopy of crystals activated by rare earth and transition metal ions, Ekaterinburg-Zarechnyi, Russia, September 22-25, 2004, p. 5.
8. G. Draganescu, M.G. Brik, C.N. Avram, N.M. Avram, "Non-radiative transitions in anharmonic model", Abstracts of the XII Feofilov symposium on spectroscopy of crystals activated by rare earth and transition metal ions, Ekaterinburg-Zarechnyi, Russia, September 22-25, 2004, p. 16.
9. M.G. Brik, N.M. Avram, C.N. Avram, K. Ogasawara, T. Ishii, I. Tanaka, "Paramagnetic susceptibility and EPR g-factors simulations from crystal field effects for trivalent lanthanides in $LiYF_4$", Conference Program and Abstracts of the Asia Pacific EPR/ESR symposium, India, Bangalore, November 21-25, 2004, p.77-78.
10. M.G. Brik, T. Ishii, K. Ogasawara, "Calculations of the Cr^{4+} and V^{3+} energy level schemes and absorption spectra in laser crystals", First Conference on Advances in

Optical materials, Tucson, Arizona, USA, October 12-15, 2005. Delegate Manual, paper O19.

11. M.G. Brik, C.N. Avram, N.M. Avram, "Calculations of spin Hamiltonian parameters and analysis of trigonal distortions in $LiSr(Al,Ga)F_6:Cr^{3+}$ crystals", Book of Abstracts of the VII Latin American Workshop on Magnetism, Magnetic Materials and Their Applications, Reñaca, Chile, December 12–16, 2005, p. 73.
12. A. Majchrowski, K. Ozga, A. Suchocki, T. Lukasiewicz, I.V. Kityk, M.G. Brik, I. Sildos, A. Slezak, "Spectroscopic study of Pr-doped BiBO glass and $Ca_4GdO(BO_3)_3$ single crystals", Book of Abstracts of the First International Conference on Rare Earth Materials REMAT, Karpacz, Poland, September 21–26, 2008, p. O4.
13. M.G. Brik, I. Sildos, V. Kiisk, "Ab-initio calculations of the optical properties of pure and Sm^{3+}-doped anatase and rutile TiO_2", Book of abstracts of the 2nd International Conference on Physics of Optical Materials and Devices ICOM 2009, Herceg Novi, Montenegro, August 26 – August 30 2009. P. 53.
14. M.G. Brik, "Modeling of Optical Properties of 3d and 4f Ions", 216th ECS Meeting - Vienna, Austria. October 4 - October 9, 2009 (**Invited Talk**)
15. M.G. Brik, I. Sildos, V. Kiisk, J. Kikas, "*Ab-initio* modeling of optical and electronic properties of pure and rare-earth ions doped wide-gap crystals under varying hydrostatic pressure", Book of abstracts of International Conference "Functional materials and nanotechnologies FM&NT 2010", Riga, Latvia, March 16–19, 2010, P. 34.
16. M.G. Brik, I. Sildos, V. Kiisk, "Ab initio and semi-empirical modeling of physical properties of pure and doped optoelectronic materials", Abstract Book of the 17th International Conference on Dynamical Processes in Excited States of Solids DPC'10, Argonne, USA, June 20–25, 2010, P. 99 (**Invited Talk**).
17. M.G. Brik, "Electronic and optical properties of $CuXS_2$ (X = Al, Ga, In) and $AgGaS_2$ semiconductors from first-principles calculations", Program and Abstract of the 4th International Conference on Optical, Optoelectronic and Photonic Materials and Applications, August 15–20, 2010, Budapest, Hungary, P. 112.
18. M.G. Brik, I. Sildos, C.-G. Ma, V. Kiisk, "*Ab initio* Calculations of Electronic, Optical, Elastic Properties and Microscopic Treatment of Crystal Field Effects for Some Cubic Crystals", Book of Abstracts of the International Conference "Functional materials and nanotechnologies FM&NT 2011", April 5 – 8 2011, Riga, Latvia. P. 68.

19. M.G. Brik, "Ab initio calculations of structural, electronic, optical and elastic properties of Cs*X*Br_3 (*X*=Ca, Ge, Sn)", 220th Electrochemical Society Meeting, October 9 – 14, 2011, Boston, USA, Abstract #1825.

8. List of publications included into the present habilitation thesis

SEMI-EMPIRICAL AND FIRST PRINCIPLES CALCULATIONS OF OPTICAL PROPERTIES OF 3*d* AND 4*f* IONS IN CRYSTALS

Subjects of publications:

A. Crystal field analysis of the energy levels of transition metall ions in crystals

1. E. Cavalli, A. Belletti, M.G. Brik, "*Optical spectra and energy levels of the Cr^{3+} ions in MWO_4 (M= Mg, Zn, Cd) and $MgMoO_4$ crystals*", Journal of Physics and Chemistry of Solids 69 (2008) 29–34.

   My contribution to this publication consisted of performing all calculations, processing the obtained results, and participation in the preparation of the manuscript. I estimate my contribution to 50%.

2. M.G. Brik, Y.Y. Yeung, "*Semi-ab initio calculations of superposition model and crystal field parameters for Co^{2+} ions using the exchange charge model*" Journal of Physics and Chemistry of Solids 69 (2008) 2401–2410.

   My contribution to this publication consisted of performing all calculations of the crystal field parameters and energy levels, analysis of the obtained results, and participation in the preparation of the manuscript. I estimate my contribution to 60%.

3. M.G. Brik, N.M. Avram, "*Microscopic analysis of the crystal field strength and electron-vibrational interaction in cubic $SrTiO_3$ doped with Cr^{3+}, Mn^{4+} and Fe^{5+} ions*", Journal of Physics: Condensed Matter 21 (2009) 155502.

   My contribution to this publication consisted of performing all crystal field calculations, discussion of the obtained results, writing the manuscript and communicating it to the journal. I estimate my contribution to 75%.

4. M.G. Brik, A.M. Srivastava, N.M. Avram, "*Comparative analysis of crystal field effects and energy level scheme of six-fold coordinated Cr^{4+} in the pyrochlores, $Y_2B_2O_7$ (B=Ti^{4+}, Sn^{4+})*", Journal of Luminescence 131 (2011) 54–58.

My contribution to this publication consisted of performing all crystal field calculations, comparison of the obtained results with the experiments and participation in the manuscript preparation. I estimate my contribution to 50%.

5. M.G. Brik, A.M. Srivastava, N.M. Avram, "*Comparative analysis of crystal field effects and optical spectroscopy of six-coordinated Mn^{4+} ion in the $Y_2Ti_2O_7$ and $Y_2Sn_2O_7$ pyrochlores*", Optical Materials 33 (2011) 1671–1676.

My contribution to this publication consisted of performing all crystal field calculations, fitting the emission band shapes and discussion of the obtained results along with participation in the manuscript preparation. I estimate my contribution to 60%.

B. First-principles calculations of the optical properties of impurity ions in crystals

6. M.G. Brik, "*A complex first-principles study of the L2,3-edge XANES spectra and crystal field effects for divalent 3d-ions in cubic ZnS*", Journal of Physics and Chemistry of Solids 69 (2008) 2568–2577.
7. M.G. Brik, "*Complex study of the crystal field splitting, "ligand - impurity ion" charge transfer transitions and high lying 4f – 6s intraconfigurational transitions for all trivalent lanthanides in Cs_2NaYCl_6 crystal*", Journal of Alloys and Compounds 454 (2008) 38–45.

Since in both papers I am the single author, my contribution is 100%.

C. Non-radiative transitions and electron-vibrational interaction for 3d ions in crystals

8. M.G. Brik, N.M. Avram, C.N. Avram, "Jahn-Teller Effect for 3d Ions (Orbital Triplets in a Cubic Crystal Field", in: "The Jahn-Teller Effects: Fundamentals and Implications for Physics and Chemistry", Editors H. Köppel, D.R. Yarkony, H. Barentzen, Springer, 2010, pp.347–370.

My contribution to this publication consisted of performing fitting the related Jahn-Teller effect calculations and participation in the manuscript preparation. I estimate my contribution to 50%.

D. Ab initio calculations of the structural, electronic, optical and elastic properties of pure and doped crystals

9. M.G. Brik, "*First-principles study of the electronic and optical properties of $CuXS_2$ (X = Al, Ga, In) and $AgGaS_2$ ternary compounds*", Journal of Physics: Condensed Matter 21 (2009) 485502.

   Since I am the single author of this publication, my contribution is 100%.

10. A.M. Srivastava, M.G. Brik, "*Comparative ab initio study of electronic, optical and chemical bonding properties of pyrochlores, $Y_2B_2O_7$ ($B=Ti^{4+}$, Sn^{4+})*", Journal of Luminescence 130 (2010) 2368–2376.

    My contribution to this publication consisted of performing ab initio calculations, preparing the plots and diagrams, along with participation in the manuscript preparation. I estimate my contribution to 70%.

11. M.G. Brik, I. Sildos, V. Kiisk, "*First-principles calculations of optical and electronic properties of pure and Sm^{3+} -doped TiO_2*", Physica B 405 (2010) 2450–2456.

    My contribution to this publication consisted of performing ab initio calculations, preparing the plots and diagrams, writing the manuscript and communicating it to the journal. I estimate my contribution to 75%.

12. M.G. Brik, A. Majchrowski, L. Jaroszewicz, A. Wojciechowski, I.V. Kityk, "*Spectroscopy of $YAl_3(BO_3)_4:Cr^{3+}$ crystals following first principles and crystal field calculations*", Philosophical Magazine 90 (2010) 4569–4578.

    My contribution to this publication consisted of performing all crystal field and ab initio calculations, preparing the plots and diagrams, and participation in the manuscript writing. I estimate my contribution to 50%.

13. M.G. Brik, I. Sildos, V. Kiisk, "*Calculations of physical properties of pure and doped crystals: Ab initio and semi-empirical methods in application to $YAlO_3:Ce^{3+}$ and TiO_2*", Journal of Luminescence 131 (2011) 396–403.

    My contribution to this publication consisted of performing ab initio calculations, preparing the plots and diagrams, writing the manuscript and communicating it to the journal. I estimate my contribution to 75%.

14. M.G. Brik, "*Electronic, optical and elastic properties of $CuXS_2$ (X=Al, Ga, In) and $AgGaS_2$ semiconductors from first-principles calculations*", Physica Status Solidi C 8 (2011) 2582–2584.

    My contribution to this publication is 100%.

15. M.G. Brik, C.-G. Ma, "*First-principles studies of the electronic and elastic properties of metal nitrides XN (X = Sc, Ti, V, Cr, Zr, Nb)*", Computational Materials Science 51 (2012) 380–388.

My contribution to this publication consisted of performing ab initio calculations, preparing the plots and diagrams, writing the manuscript and communicating it to the journal. I estimate my contribution to 75%.

The statements of all co-authors of the above-mentioned papers, which indicate contribution of the co-authors, are enclosed.

9. Summary of research work

9.1 Summary of scientific results obtained before getting PhD degree

From my third year of study at the physical faculty of Kuban State University (KubSU) in Krasnodar I had been involved into the students' research work. As a result, I participated in the All-Union (USSR) students' conferences on physics (Novosibirsk, 1991) and physical optics (Tomsk, 1991). At the latter I was awarded the first degree diploma for one of the best talks. From September 1992 till November 1995 I had been taking the Postgraduate course at the Experimental Physics Department of KubSU. My PhD thesis was devoted to the theoretical calculations of the energy levels schemes of impurity ions in laser crystals and development of a model for non-radiative transitions between their energy levels. My thesis was supervised by late Prof. Dr. Sci. V.F. Pisarenko; I also worked in a close contact with late Dr. A.G. Avanesov and Dr. V.V. Zhorin (formerly with KubSu, then with Argonne National Laboratory, currently with the Economics Department of University of Chicago, USA). The main results of my thesis were presented at several conferences (conferences with my personal participation and presentation are in bold):

- X Feofilov symposium on spectroscopy of crystals activated by rare-earth and transitional ions, Saint-Petersburg, Russia, June 1995.
- **IX International Conference ICPS'94, Saint-Petersburg, Russia, August 1994.**
- III International School "Excited States of Elements", Wroclaw, Poland, 1994.
- **International Conference on Luminescence, Moscow, Russia, November 1994.**

The main results of the PhD thesis were as follows:

- demonstration of pronounced dependence of the impurity ions' energy levels on momentary ligands' configuration. From a thorough analysis of different position of ligands, dependence of the impurity's energy levels on magnitudes of the normal vibrational modes for the tetrahedral and octahedral complexes.
- development of a new model of the energy levels crossing in the theory of non-radiative transitions (NRT). According to this model, the NRT takes place when purely electronic levels of an impurity ions are crossing due to the ligands' thermal vibrations. The analytical expression for the temperature dependence of the NRT probability was obtained in the harmonic approximation and successfully applied to the case of the Cr^{4+} ion in $Y_3Al_5O_{12}$ (its $^3T_2$ - $^3A_2$ transition) (M.G. Brik, "*Non-radiative transitions in the model of energy levels crossing*", Proc. of the IX Int. Conf. ICPS'94, Saint-Petersburg, Russia, 1994, p.13–19).
- establishment of a close connection between the exchange charge model of crystal field and NRT processes, including previously developed linear theory of the electron-vibrational interaction. The case study was well-known system $Al_2O_3:Cr^{3+}$, and the temperature dependence of the $^4T_2$-$^4A_2$ NRT has been studied and compared to the available experimental data.

During my PhD study I co-supervised the student's research projects and gave some lectures on selected topics of theory of luminescence and group theory for the fifth year students.

The dissertation has been successfully defended on November 23, 1995, and the scientific degree of Candidate of Physical and Mathematical Sciences was confirmed by the All-Russian Committee on Scientific Degrees and Titles on February 9, 1996.

9.2 Summary of scientific results obtained after getting PhD degree

From May 1996 till September 1997 I was employed as a Junior Researcher at the Experimental Physics Department of KubSU. I continued my studies of the electron-vibrational interaction and NRT in crystals doped with 3d ions. The main results of that year were presented at the International Conference on Luminescence in Prague (1996) and published in one article (M.G. Brik, V.V. Zhorin, J. Lumin. 72–74 (1997) 149–151).

Since September 1997 till March 1998 I had been working as a Senior Lecturer at the General Physics Department, KubSU. I was promoted to the Associate Professor position in March 1998, and on February 20, 2001 the Docent certificate was issued by the Russian Ministry of Education. From September 1997 till September 2000 I have had an extensive teaching load. The total number of academic hours was 780 per year (it was the normal load for full-time position at that time in Russia). I had prepared several lecture courses, e.g. Mechanics (General Physics); Applied Mechanics; Introduction to the Quantum Theory of Atoms and Molecules; Theory of Atomic Spectra; practical classes on all of these courses and laboratories on mechanics and optics. I also supervised a number of the students research and diploma projects.

My scientific work at that time was a combination of my previous activities related to the 3d elements (M.G. Brik, D.G. Shchekoldin, Optics and Spectroscopy 84 (1998) 683–684; A.G. Avanesov, M.G. Brik, E.N. Tumayev, J. Lumin. 92 (2001) 133–137) and beginning of a new for me topic - studies of the rare earth elements in laser crystals (V.A. Lebedev, V.F. Pisarenko, N.V. Selina, A.A. Perfilin, M.G. Brik, Opt. Mater. 14 (2000) 121–126). I do not mention here several papers published in local Russian journals.

In addition to teaching and research, during those three years I also prepared two manuals for students: i) M.G. Brik, I.D. Bregeda, M.P. Matveyakin, “Methods of treatments of experimental results in physical laboratory” (in Russian), Krasnodar, Kuban State University, 1997, 73 pages, and ii) M.G. Brik, I.D. Bregeda, M.P. Matveyakin, “Mechanics: problems with solutions” (in Russian), Krasnodar, Kuban State University, 2000, 112 pages.

In September 2000 I was invited by Prof. M.M. Avram (West University of Timisoara, Romania) to visit his research group and deliver there a series of seminars (4 altogether) on theory of crystal field and electron-vibrational interaction for impurity ions. It turned out to be a start of a very long and fruitful scientific collaboration.

In October 2000 I moved to Asmara, Eritrea, where I took an Associate Professor position at the Department of Physics of Asmara University. I stayed there until the end of December of 2001. My main job there was teaching: I taught statistical physics, electrodynamics, quantum mechanics. I attended the CLEO-Europe conference in Munich, Germany (June 2001) and XI Feofilov symposium in Kazan, Russia (October 2001), where I had several poster presentations. Two manuals were published in 2001 for the students of Asmara University: i) M.G. Brik, S.S. Kotelnikov, M.Kahsay, “Physics 206: Electricity and Optics. Laboratory Manual”, University of Asmara, Asmara, 2001, 56 pages, and ii) M.G.

Brik, S.S. Kotelnikov, “Kinematics: problems with solutions”, University of Asmara, Asmara, 2001, 26 pages.

From the end of December of 2001 till the end of December of 2002 I had been working as a Visiting Scientist at the Chemical Physics Department, Weizmann Institute of Science, Rehovot, Israel. My research was focused mainly on theoretical studies of the absorption and emission spectra of polyatomic molecules: modeling of the emission band shape with taking into account all normal modes and decrease of the normal modes frequencies in the excited state (Reuven Ianconesu, Mikhail G. Brik, Eli Pollak, New Journal of Physics 7 (2005) 22). Continuation of the crystal field studies of the 3d ions in laser crystals (Cr^{3+} in Al_2O_3 and $LiCaAlF_6$) resulted in several presentations at the International Conference on Luminescence in Budapest in 2002 and "Advanced Solid State Lasers" in Montreal (presented by my co-authors).

From March 2003 till July 2007 I was working in Japan, in Fukui Institute for Fundamental Chemistry, Kyoto University, and (between July 2005 and October 2006) simultaneously in the Kwansei Gakuin University, Sanda, Japan. During my Japanese period I was involved into the *ab initio* and crystal field calculations of the energy levels and absorption spectra of the rare earth and transition metal ions in crystals. In addition, the XANES (X-ray Absorption Near Edge Structure) spectra for the 3d elements have been modeled from the *ab initio* point of view. The DV-ME (discrete variational multi-electron) method was used as the main tool for the *ab initio* calculations. The method is based on the numerical solution of the Dirac equation; the program for calculations had been developed by Prof. S. Adachi and Assoc. Prof. K. Ogasawara. The main results obtained during those 4 years were as follows:

- extension of the standard Dieke's diagram to the UV and VUV spectral regions by calculating *complete* energy levels schemes for the $4f^N$ and $4f^{N-1}5d$ electronic configurations of all trivalent lanthanides;

- systematic analysis, simulation and assignment of the 4f-5d spectra for a number of trivalent lanthanides (Ce^{3+}, Pr^{3+}, Nd^{3+}, Ho^{3+}, Er^{3+}, Tm^{3+}) in $LiYF_4$;

- extension of the energy levels crossing model in the theory of NRT to anharmonic approximation (Morse oscillator);

- development of a series of computer programs for calculating the crystal field parameters and diagonalization of the crystal field Hamiltonians for all $3d^N$ electron configurations with subsequent application to the analysis of the absorption spectra of laser crystals doped with the transition metal ions;

- development of a series of computer programs for calculations of the doubly reduced matrix elements of the unit tensor operators required for applications of the Judd-Ofelt theory (both standard and modified) for all trivalent lanthanides.

The summary of the performed first principles calculations was presented in the book "First-principles Calculations of Spectral Properties of Rare-Earth and Transition Metal Ions in Crystals", Editors Mikhail G. Brik and Kazuyoshi Ogasawara, Transworld Research Network, 2006, and in the book chapter K. Ogasawara, S. Watanabe, H. Toyoshima, M.G. Brik, "First principles calculations of $4f^n - 4f^{n-1}5d$ transition spectra", Handbook on the Physics and Chemistry of the Rare Earths, Vol. 37, North Holland, Amsterdam. Edited by K.A. Gschneidner, Jr., J.-C.G. Bünzli and V.K. Pecharsky, 2007, pp. 1-59.

In 2006 I have been awarded the Dragomir Hurmuzescu Award of the Romanian Academy (together with N.M. Avram, C.N. Avram, and I. Tanaka).

From July 2007 I have been working in the Institute of Physics, University of Tartu, first as a Guest Professor (until July 2008), then as an Extraordinary Senior Researcher and, finally, since February 2010, as a Professor of Computational Materials Science. My current research interests are focused on the following topics: i) *ab initio* calculations of the electronic, optical and elastic properties of pure and doped crystals; ii) crystal field analysis of the impurity ions' energy levels in crystals; iii) simultaneous application of the *ab initio* methods and crystal field theory to the same materials with the aim of getting complementary information about a studied material; iv) microscopic studies of the crystal field effects - dependence of the crystal field strength on interionic distances and its manifestation in the optical spectra; v) studies of the electron-vibrational interaction for the transition metal and rare earth ions.

In addition to the above-mentioned research activities, I teach a lecture course "Spectroscopy of atoms, molecules and crystals" for the MSc and PhD students of the University of Tartu, which has been published separately in the form of a textbook: M.G. Brik, I. Sildos, V. Kiisk, "Introduction to spectroscopy of atoms, molecules and crystals", Tartu University Press, 2008, 234 p. I have also been a co-supervisor of one successfully defended PhD thesis: Sven Lange, Doctor's Degree, 2010, supervisors Ilmo Sildos, Mikhail G. Brik, Spectroscopic and Phase-stabilization Properties of Pure and Rare-earth Ions Activated ZrO_2 and HfO_2,University of Tartu, Faculty of Science and Technology, Institute of Physics, University of Tartu.

Currently I supervise two postdoctoral researchers: Dr. Chong-Geng Ma and Dr. V. Krasnenko. I am the supervisor of the research project funded by the Estonian Science

Foundation (September 2010 - September 2013; the total budget 100,341.29 EUR, or 1,500,000 former Estonian Kroons) and Dr. Ma is the principal investigator in this project.

Presently I am involved into three research projects: i) Design of advanced nanostructured materials with tailored properties for novel laser and light sources; ii) Temperature- and light-controlled defectiveness of metal oxides for application in optical gas sensing; iii) Low-dimensional structures and their applications. Information about this projects can be found at:
https://www.etis.ee/portaal/isikuCV.aspx?TextBoxName=brik&PersonVID=55817&lang=en&FromUrl0=isikud.aspx

In 2008 I was appointed as an Honorary Associate Professor, and in September of 2011 I was appointed as an Honorary Professor of the Department of Science and Environmental Studies of The Hong Kong Institute of Education.

9.2.1 Scientific achievements representing the subject of the habilitation thesis

Semi-empirical and first principles calculations of optical properties of 3*d* and 4*f* ions in crystals

The ions with unfilled *d* and *f* electron shells in crystals (either as impurities or initially existing as a part of the crystal lattice in the so-called self-doped crystals) are extensively studied during the last several decades. The reason is that these materials possess unique physical (optical, magnetic, electric, non-linear etc) properties, which make them suitable for numerous applications such as solid-state laser active elements, luminescent materials, optical detectors, non-linear optical devices etc. A large number of the energy levels with different relative positions, especially for the ions from the middle parts of the transition metal (TM) and rare-earth (RE) ion series, in a combination with different host materials providing the crystal fields of various symmetries and strengths make the optical absorption spectra of these ions extremely reach in the number of the absorption bands in wide spectral regions, from infrared (IR) to ultraviolet (UV) and vacuum ultraviolet (VUV).

The present habilitation thesis is devoted to the further development and systematic applications of several semi-empirical and first-principles methods to the calculations of the energy levels, absorption spectra (in the optical and X-ray spectral regions), probabilities of the non-radiative transitions, microscopic treatment of the crystal field effects and electron-

vibrational interaction in a large number of crystals containing the TM and RE ions. The performed systematic calculations allowed to reveal common trends between various types of host materials and impurities, which are discussed in the dissertation. The basis of the habilitation thesis is formed by the above given list of 15 papers, grouped into 4 categories A, B, C, and D.

The new results obtained in the dissertation can be grouped as follows:

1. The exchange charge model (ECM) of crystal field (CF) [1] (developed and initially applied mainly to the RE ions) has been systematically applied to an analysis of the optical spectra of a large number of crystals doped with 3*d* ions [2,3,4,5,6,7,8,9,10,11,12,13,14,15,16]. Along with the crystal field parameters (CFP) and energy levels calculations, the symmetry aspects of the impurity centers and convergence properties of the crystal lattice sums have been thoroughly considered [9,11,14]. A series of the original MAPLE codes have been written to calculate the CFP values and diagonalize the CF Hamiltonians (including the spin-orbit interaction and Trees correction terms) for ions with any number of *d*-electrons in a crystal field of an arbitrary symmetry **(papers A1, A3-A5).**

2. For the first time the two independent CF models – the ECM and the superposition model (SM) – have been linked together [12]. Using the distance dependence of the CF invariants, the SM parameters (the power exponents and intrinsic parameters) have been reliably calculated, but not varied freely as has been done previously **(paper A2).**

3. For the first time the discrete variational multielectron method (DVME) [17] has been systematically applied in the following cases:

a) computer calculations of the energy levels and absorption spectra (in the optical and X-ray regions) of 3*d* and 4*f* ions in a number of crystals [18,19,20]. The covalent effects, molecular orbitals (MO) compositions, their relative locations were considered in various complexes; dependence of the above-mentioned effects on the central ion oxidation state, its atomic number and the nature of ligands has been explored **(paper B6)**;

b) microscopic analysis of the crystal field effects and "impurity ion – ligand" charge transfer (CT) transitions for the transition metal and RE ions in cubic elpasolites has been performed [21,22] **(paper B7).**

4. A thorough analysis of the dynamical Jahn-Teller effect in the $^4T_{2g}$ state of $3d^3$ ions (V^{2+}, Cr^{3+}, Mn^{4+}) has been performed using the Ham effect (quenching of the spin-orbit splitting) and geometry of the ligands configurations in the excited state. In this way, the magnitudes of the ligands' displacements as the result of the combined effect of the a_{1g} and e_g

modes of the octahedral complex were calculated and the cross-sections of the potential energy surfaces were plotted for a number of octahedral complexes [23,24,25] **(paper C8).**

5. Detailed density functional theory (DFT) based studies (as implemented in the plane wave based CASTEP program) of the structural, electronic, optical and elastic properties of a number of pure and doped compounds were performed [26,27,28,29,30,31,32,33,34,35,36,37]. For the pure crystals, the pressure effects have been modeled to analyze how the interionic distances, band gaps, electron density distributions vary with applied hydrostatic pressure. For the doped crystals, thorough attention was paid to the modifications of the electronic and optical properties of a crystal after doping. In particular, positions of the lowest impurity ion's energy levels in the host's band gap were estimated for a number of systems with already existing and yet potential applications. For the first time, the an initio methods and crystal field theory have been applied simultaneously to the same systems (like $YAlO_3$:Ce^{3+}, $YAl_3(BO_3)_4$:Cr^{3+}, CdI_2:Ni^{2+}) to get a complementary picture of the electronic and optical properties of these materials. Such a combination of two different approaches is a powerful tool for deeper studies of the doped crystals. An original technique of treating the microscopic crystal field effects by following the distribution of peaks of the 3d electrons' density of states was developed and successfully tested. Particular attention has been paid to the *ab initio* modeling of the pressure effects and their influence on the structural, electronic, optical and elastic properties of different crystals. Elastic anisotropy of cubic crystals (dependence of the Young's moduli on the direction in the crystal has been considered **(papers D9-D15).**

9.3. General summary

As a result of my work on the topic of this habilitation thesis, from 2003 and until now more than 160 papers have been published in the international scientific journals (listed in the ISI/Scopus databases); in 77 papers I was the first or the single author. About 100 presentations at the international conferences have been given (including the invited talks at the 216th Electrochemical Society Meeting (Vienna, Austria, 2008), 17th International Conference on Dynamical Processes in Excited States of Solids DPC'10 (Argonne, USA, 2010).

Short-time research visits to my colleagues' laboratories and research groups (almost during every visit the seminars were organized for staff members of those groups) were made; e.g. Institute of Physics, Polish Academy of Sciences (Warsaw, Poland); Czestochowa University of Technology (Chestochowa, Poland); University of Texas at San Antonio,

Argonne National Laboratory, GE Global Research (all in the USA); Universidad de Guanajuato and Centro de Investigaciones de Optica (Mexico); Institute for Laser Physics (Hamburg, Germany); Universities of Verona and Padova (Italy); West University of Timisoara (Timisoara, Romania); The Hong Kong Institute of Education (Hong Kong, China); The Australian National University (Canberra, Australia); University of Canterbury (Christchurch, New Zealand); Assiut University (Assiut, Egypt).

Acknowledgments

This habilitation thesis represents a summary of my work in the last 8 years, which was done at Fukui Institute for Fundamental Chemistry, Kyoto University, Japan (2003 – 2007) and at the Institute of Physics, University of Tartu, Estonia (from 2007 till present). These years were filled with interesting work and exciting meetings and contacts with my numerous colleagues (many of them became my good friends), to whom I am very grateful:

Profs. Nicolae M. Avram, Calin N. Avram, Georghe E. Draganescu: for their encouraging support and absolute friendship. My international career began with my first visit to the West University of Timisoara in 2000, and I always recollect with greatest pleasure our walks in Timisoara and Buziash, as well as our meetings with Prof. N.M. Avram in many other countries.

Prof. Isao Tanaka – for introducing me into the field of the *ab initio* calculations, giving me an unprecedented freedom in choosing the topics for research while I was in Kyoto and supporting me in all my doings.

Prof. Peter A. Tanner – for turning my attention to cubic elpasolites and for his friendship, unbelievable strength and sense of humor.

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Prof. Andrzej Suchocki and Dr. Agata Kaminska – for their friendship, support and my involvement into exciting projects on high-pressure studies of optical spectra of rare earth ions in various crystals.

Prof. Iwan V. Kityk – for his friendship and amazing research activity.

Dr. Alok M. Srivastava – for his friendship and his ability to find interesting and unusual experimental results, which wait for their turn to be explained and modeled theoretically.

Profs. Marco Bettinelli and Enrico Cavalli – for their friendship and interesting joined research projects.

Prof. Michael F. Read – for stimulating discussions on spectroscopy of rare earth ions and for his hospitality during my visits to New Zealand.

With all these people (and many others, whom I simply do not have enough space to mention), I enjoyed very interesting scientific and personal discussions and conversations, meeting them in different places all over the globe.

At last (but not at least) I thank family for their patience and tolerance. Finally, I am very much indebted to my mother and my late father, to whom I would like to dedicate this thesis.

Tartu, Estonia, 17.III.2012

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date Signature

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