europass Curriculum vitae

PERSONAL INFORMATION

Dmitry Bocharov

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Date of birth 30/10/1981

WORK EXPERIENCE

01/04/2002–Present
Researcher (Engineer prior to 10/2006, Research assistant prior to 9/2012)
Institute of Solid State Physics, Department of Theoretical Physics and Computer Modeling, Riga (Latvia)

01/02/2013–Present
Docent (Lecturer prior to 02/2014)
Transport and Telecommunication Institute, Riga (Latvia)

01/04/1999–Present
Non-formal education project manager
NGO UNESCO-Club “Culture. Tolerance. Friendship.”, Riga (Latvia)

01/09/2014–31/08/2015
SCIEX programme visiting fellow
Paul Scherrer Institute, Villigen (Switzerland)

05/03/2013–31/12/2014
Physicist
Faculty of Physics and Math, University of Latvia, Riga (Latvia)

01/10/2013–31/01/2014
Researcher
Faculty of Physics and Math, University of Latvia, Riga (Latvia)

01/12/2009–30/11/2012
Researcher
Faculty of Computing, University of Latvia, Riga (Latvia)

01/11/2007–31/12/2007
Research assistant
Faculty of Physics and Math, University of Latvia, Riga (Latvia)

EDUCATION AND TRAINING

01/10/2006–24/01/2012
Dr.phys., thesis “First principles simulations of surface properties and reactivity of nitride nuclear fuels” (supervisor Dr.chem. Yuri F. Zhukovskii)
University of Latvia, Riga (Latvia)

01/09/2004–30/06/2006
Master of natural sciences in physics, thesis “Quantum chemical interpretation of x-ray absorption spectra in perovskite type compounds” (supervisor Dr.phys. Aleksejs Kuzmins)
University of Latvia, Riga (Latvia)

01/09/2000–30/06/2004

Bachelor of natural sciences in physics

Latvijas Universitāte, Riga (Latvia)

PERSONAL SKILLS

Mother tongue(s): Russian

Other language(s)

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
Latvian	C1	C1	C1	C1	C1
English	B2	B2	B2	B2	B2

Levels: A1 and A2: Basic user - B1 and B2: Independent user - C1 and C2: Proficient user
Common European Framework of Reference for Languages

Organisational / managerial skills

04.2016-to date: Member of ISSP UL scientific council

2002-to date: Organizing committee member of the Latvian Open Physics Olympiad for high-school students (in 2005-2007, 2011-2013 and 2016 as Olympiad coordinator), organizing committee member of the Latvian Physics Olympiad for high-school students (2012-to date) and Young Researcher School in Physics (2010-to date)

2003-to date: Coordinator of Riga Intellectual Games Championship for High School students

Job-related skills

12.2012-to date Expert of Latvian Council of Science

Publications:

Peer-reviewed journals:

1. R.A. Evarestov, A.V. Bandura, M.V. Losev, E.A. Kotomin, Yu.F. Zhukovskii, and D. Bocharov, A first principles DFT study in UN bulk and (001) surface: comparative LCAO and PW calculations. - J. Comput. Chem., 2008, 29, p. 2079-2087.

2. D. Bocharov, A. Kuzmin, J. Purans, and Yu.F. Zhukovskii, Quantum chemistry studies of the O K-edge X-ray absorption in WO_3 and AWO_3. - SPIE Proceedings (Proc. AOMD-6, Riga, Latvia, 2008), 2008, 71420T (p. 1-9).

3. N. Zaporina, O. Doynikova, A. Krumina, D. Bocharov, and J. Grabis, Methods of electron microdiffraction and X-ray analysis in structure study of nanodisperse partially stabilized ZrO_2 powders. - J. Surf. Investigation: X-ray, Synchrotron and Neutron Techniques, 2009, 3, p. 464-467.

4. Yu.F. Zhukovskii, D. Bocharov, E.A. Kotomin, R.A. Evarestov, and A.V. Bandura, First principles calculations of oxygen adsorption on the UN(001) surface. - Surf. Sci., 2009, 603, p. 50-53.

5. Yu.F. Zhukovskii, D. Bocharov, and E.A. Kotomin, Chemisorption of a molecular oxygen on the UN (001) surface: *ab initio* calculations. - J. Nucl. Mater., 2009, 393, p. 504-507.

6. N. Zaporina, J. Grabis, V.N. Timofeev, andD. Bocharov, Microstructural investigations of multicomponent SiC/Si_3N_4-Al_2O_3-Y_2O_3 nanopowders. - Latv. J. Chem., 2010, No 1, p. 33-38.

7. D. Bocharov, D. Gryaznov, Yu.F. Zhukovskii, and E.A. Kotomin, DFT calculations of point defects on UN(001) surface. - Surf. Sci., 2011,605, p. 396-400.

8. D. Bocharov, D. Gryaznov, Yu.F. Zhukovskii, and E.A. Kotomin, *Ab initio* modeling of oxygen impurity atom incorporation into uranium mononitride surface and subsurface vacancies, J. Nucl. Mater., 2011, 416, p. 200-204.

9. Yu.F. Zhukovskii, D. Bocharov, D. Gryaznov, and E.A. Kotomin, 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 Acess Publishers), 2012, p. 95-122.

10. 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).
11. N. Zaporina, J. Grabis, M. Maiorov, A. Krumina, G. Heidemane, D. Bocharov, Nanodisperse nickel ferrite: methods of production, structure and magnetic properties, Latv. J. Chem., 2012, No. 1/2, p. 99–104.

12. A. Sorokine, D. Bocharov, S. Piskunov, and V. Kashcheyevs , Electronic charge redistribution in $LaAlO_3$ (001) thin lms deposited at $SrTiO_3$ (001) substrate: First-principles analysis and the role of stoichiometry. - Phys. Rev. B, 2012, 86, 155410 (p. 1-10).

13. D. Bocharov, D. Gryaznov, Yu.F. Zhukovskii, and E.A. Kotomin, *Ab initio* simulations of oxygen interaction with surfaces and interfaces in uranium mononitride. - J. Nucl. Mater., 2013, 435, (p. 102–106).

14. A. Anspoks, D. Bocharov, J. Purans, F. Rocca, A. Sarakovskis, V. Trepakov, A. Dejneka, and M. Itoh, Local structure studies of $SrTi^{16}O_3$ and $SrTi^{18}O_3$. - Phys. Scr., 2014, 89, 044002 (p. 1-5)

15. S. Piskunov, O. Lisovski, J. Begens, D. Bocharov, Yu.F. Zhukovskii, M. Wessel, and E. Spohr, C-, N-, S-, and Fe-doped TiO_2 and $SrTiO_3$ nanotubes for visible-light-driven photocatalytic water splitting: Prediction from first principles. - J. Phys. Chem. C, 2015, 119, p. 18686−18696.

16. A. Chesnokov, O. Lisovski, D. Bocharov, S. Piskunov, Yu.F. Zhukovskii, M. Wessel, and E. Spohr, *Ab initio* simulations on N and S co-doped titania nanotubes for photocatalytic applications. - Phys. Scr., 2015, 90, 094013 (p.1-7).

17. A. Anspoks, J. Timoshenko, D. Bocharov, J. Purans, F. Rocca, A. Sarakovskis, V. Trepakov, A. Dejneka, and M. Itoh, Local structure studies of Ti for $SrTi^{16}O_3$ and $SrTi^{18}O_3$ by advanced X-ray absorption spectroscopy data analysis. - Ferroelectrics, 485, 2015, p. 42–52.

18. S. Piskunov, P.A. Žguns, D. Bocharov, A. Kuzmin, J. Purans, A. Kalinko, R.A. Evarestov, S.E. Ali, and F. Rocca, Interpretation of unexpected behavior of infrared absorption spectra of ScF_3 beyond the quasiharmonic approximation. - Phys. Rev. B, 2016, 93, 214101 (p. 1-9).

19. D. Bocharov, M. Krack, A. Kalinko, J. Purans, F. Rocca, S.E. Ali, and A. Kuzmin, Ab initio molecular dynamics simulations of the Sc K-edge EXAFS of scandium trifluoride. - J. Phys. Conf. Ser., 2016, 712, 012009 (p. 1-4).

20. J. Purans, S. Piskunov, D. Bocharov, A. Kalinko, A. Kuzmin, S.E. Ali, and F. Rocca, Local structure of perovskites ReO_3 and ScF_3 with negative thermal expansion: interpretation beyond the quasiharmonic approximation. - J. Phys. Conf. Ser., 2016, 712, 012013 (p. 1-4).

21. D. Bocharov, M. Chollet, M. Krack, J. Bertsch, D. Grolimund, M. Martin, A. Kuzmin, J.Purans, and E.A. Kotomin, Interpretation of the U L_3-edge EXAFS in uranium dioxide using molecular dynamics and density functional theory simulations. - J. Phys. Conf. Ser., 2016, 712, 012013 (p. 1-4).

22. D. Bocharov, P. Žguns, S. Piskunov, A. Kuzmin, and J. Purans, Electronic structure of cubic ScF_3 from first-principles calculations. - Low Temp. Phys., 2016, 42, p. 710-715.

23. O. Lisovski, A. Chesnokov, S. Piskunov, D. Bocharov, Yu.F. Zhukovskii, M. Wessel, and E. Spohr, Ab initio calculations of doped TiO_2anatase (101) nanotubes for photocatalytical water splitting applications. – Mater. Sci. Semicond. Process. 2016, 42, p. 138-141.

24. Yu.F. Zhukovskii, S. Piskunov, O. Lisovski, A. Chesnokov, and D. Bocharov, First principle evaluation of photocatalytic suitability for TiO_2-based nanotubes. - Chapter in a book: W. Cao (Ed.) Semiconductor Photocatalysis - Materials, Mechanisms and Applications (InTech Open Access Publishers, Croatia), 2016, p. 105-133.

25. D. Bocharov, M. Chollet, M. Krack, J. Bertsch, D. Grolimund, M. Martin, A. Kuzmin, J. Purans, and E.A. Kotomin, Analysis of the U L_3-edge X-ray absorption spectra in UO_2 using molecular dynamics simulations. - Progr. Nucl. Ener., 2017, 94, p. 187-193.

26. O. Lisovski, S. Piskunov, Yu.F. Zhukovskii, and D. Bocharov, Quantum chemical simulations of titanium dioxide nanotubes used for photocatalytic water splitting. - J. Surf. Investigation, 2017, 11, p. 78–86.

Science popularization

1. V. Fļorovs, A. Cēbers, D. Bočarovs, V. Kaščejevs, D. Docenko, Latvijas 30. atklātā fizikas olimpiāde. – “Zvaigžņotā Debess", 2005, 190, p. 63-70.

2. A. Petroveca, D. Bočarovs, Neformālās izglītības iespējas fizikā, astronomijā un matemātikā. - “Zvaigžņotā Debess", 191, p. 68-74.

3. V. Fļorovs, A. Cēbers, D. Bočarovs, V. Kaščejevs, Latvijas 31. atklātā fizikas olimpiāde. –

“Zvaigžņotā Debess", 2006, 194, p. 51-56.

4. V. Fļorovs, A. Cēbers, D. Bočarovs, D. Docenko, V. Kaščejevs, Latvijas 32. atklātā fizikas olimpiāde. – “Zvaigžņotā Debess", 2007, 197, p. 53-58.

5. V. Fļorovs, A. Cēbers, D. Bočarovs, D. Docenko, P. Nazarovs, J. Timošenko, V. Kaščejevs, Latvijas 33. atklātā fizikas olimpiāde. – “Zvaigžņotā Debess", 2008, 202, p. 43-51.

6. V. Fļorovs, A. Cēbers, V. Kaščejevs, D. Bočarovs, D. Docenko, Latvijas 34. atklātā fizikas olimpiāde. – “Zvaigžņotā Debess", 2009, 206, p. 43-48.

7. V. Fļorovs, A. Cēbers, D. Docenko, D. Bočarovs, V. Kaščejevs, Latvijas 35.atklātā fizikas olimpiāde. – “Zvaigžņotā Debess", 2011, 211, p. 40-46.

8. V. Fļorovs, A. Cēbers, D. Bočarovs, J.Timošenko, D. Docenko, and V. Kaščejevs, Latvijas 36.atklātā fizikas olimpiāde. – “Zvaigžņotā Debess", 2011, 214, p. 33-39.

9. V. Fļorovs, D. Docenko, D. Bočarovs, A. Cēbers, Latvijas 37. atklātā fizikas olimpiāde. – “Zvaigžņotā Debess", 2012, 218, p. 45-52.

10. D. Docenko, D. Bočarovs, A. Cēbers, Ļ. Dolgovs, J. Timošenko, Latvijas 38. atklātā fizikas olimpiāde. – “Zvaigžņotā Debess", 2013, 222, p. 45-51.

11. D. Bočarovs, A. Cēbers, J. Timošenko, D. Docenko, Latvijas 39. atklātā fizikas olimpiāde. – “Zvaigžņotā Debess", 2014, 226, p. 37-43.

12. D. Docenko, A. Cēbers, D. Bočarovs, J. Timošenko, Latvijas 40. atklātā fizikas olimpiāde. – "Zvaigžņotā Debess", 2015, 230, p. 42-49.

13. D. Bočarovs, J. Timošenko, D. Docenko, A. Cēbers, A. Katkevičs, Latvijas 41. atklātā fizikas olimpiāde. – "Zvaigžņotā Debess", 2016, 230, p. 41-49.

Teaching activities:

2012-2014 and 2015-to date Transport and Telecommunication Institute, Riga, Latvia, Bachelor program course "Higher mathematics"

2006-2014 Conduction of a practical work "X-ray absorption spectroscopy" at the Latvian University (in frames of "Solid state and material science laboratory" course for Master/Bachelor students)

2007 Exercises preparation for Master program course "Structure and Description of Nanomaterials" (Latvian University course Fizi5028).

Digital competence

Windows, Linux, MS Office, Mathematica, Origin, LaTeX; computational codes for materials simulations in chemistry, physics and material science (VASP, CRYSTAL, FEFF, CP2K)