CURRICULUM VITAE

Yuri F. Zhukovskii (Jurijs Žukovskis)

2.02.1949 – 22.12.2018

SCIENTIFIC DEGREES:
Dr. Chem.

DATE AND PLACE OF BIRTH:
February 2, 1949, Riga, Latvia

ADDRESS: **Institute of Solid State Physics,**
University of Latvia, 8 Kengaraga Str., LV-1063 Riga, Latvia

PHONE: 371-67187480 (office), 371-67450972 (home), 371- 28824271 (mob.)
FAX: +371-6713-2778
E-MAIL: quantzh@latnet.lv

1. MAIN RESEARCH INTERESTS:

Physics and Chemistry of Crystalline Solids,
Surface Science, Adsorption and Surface Reactivity,
Physics and Chemistry of Nanostructures,
Quantum Chemistry,
Computational Materials Science

2. EDUCATION

- *1966-75*. **B.S. + M.S. degrees**: Department of Physics and Mathematics, the University of Latvia, Riga, Latvia.
- *1993*. **Ph.D. degree (Dr. Chem.)**: Institute of Inorganic Chemistry, Latvian Academy of Sciences, Latvia, and Institute of Physics, St. Petersburg State University, Russia. Title of the Thesis: "Quantum-chemical study of water chemisorption on aluminum surface".

3. ACADEMIC AND PROFESSIONAL EXPERIENCE, SCIENTIFIC VISITS

08.1975-08.1977.	**Teacher of physics and mathematics, 67 Secondary School in Riga, Latvia**
• *09.1977-04.1980;* *05.1980-06.1986;* *07.1986-12.1993.*	Engineer, Institute of Inorganic Chemistry, Latvian Academy of Sciences, **Riga** Junior research associate, at the same Institute, Riga - **Salaspils**, Research associate, at the same Institute, **Salaspils**, **Latvia**
• *10.1988-04.1989.*	Visiting scientist, Institute of Physics at **Leningrad** State University, **Russia**.
• *01.1994-0219.95.*	Researcher, Institute of Inorganic Chemistry, Latvian Academy of Sciences, **Salaspils**.
• *08.1994-07.1995.*	Teacher of physics and mathematics, 38 Secondary School in **Riga**, **Latvia**
Since 03.1995.	**Senior researcher, Institute of Solid State Physics at University of Latvia, Riga.**
• *09.1995-03.1996;* *09.1996-01.1997.*	Visiting fellow, Laboratory of Physics at Helsinki University of Technology, **Espoo**, **Finland**.
• *09.1997-08.1999;* *10-11.2001.*	Senior visiting fellow, Centre for Chemical Physics at University of Western Ontario, **London** (Ontario), **Canada**.
• *01-02.2000.*	Visiting scientist, Centre for Materials Research at University College **London**, **UK**.
• *04-05,11.2000;* *06.2001; 10-11.2003.*	Visiting scientist, Materials Chemistry, the Ångström Laboratory at **Uppsala** University, **Sweden**.
• *03-04.2002*; *05.2004;* *09.2005; 02;10.2006;* *09.2007, 02.2008.*	Senior visiting scientist, Max Planck Institute of Solid State Research, **Stuttgart**, **Germany**.
• *06.2002; 04.2003;*	Visiting scientist, Physics Department at **Osnabrück** University, **Germany**.

06.2004.	
• *09,12.2004; 08; 12.2006; 12.2007; 06;12.2008; 02;09;12.2009; 02,06.2010; 02;06;09;12.2011; 02;06;09.2012; 02;06.2013; 06;10-11.2014; 02;06.2015; 02;06.2016.*	Visiting scientist, Scientific Research Institute of Chemistry, **St. Petersburg** State University, **Russia**.
• *02-03;06-07.2005; 04-06.2006; 02;05-07.2007; 05;09.2008; 07.2009.*	Stipend holder from National Science Foundation (NSF) for short-term visits (≤ four months annually); Visiting fellow, Materials Research Center at Northwestern University, **Evanston** (Illinois), **USA**.
• *10.2005; 05;11.2006; 10.2007; 11.2008.*	Visiting scientist, National Laboratory of **Frascati** (National Institute of Nuclear Physics), **Italy.**
• *09.2006; 03.2007; 09.2009.*	Visiting scientist, EC Institute of Transuranum Elements, **Karlsruhe**, **Germany**.
• *03;09.2007; 03;10.2008; 05;10.2009; 05;10.2010; 06;10.2011; 05;10.2012; 06;10.2013; 10.2015.*	Visiting scientist, Institute of Applied Mateirals (KIT), **Karlsruhe**, **Germany**.
• *03;05.2011; 05.2013.*	Visiting scientist, Institute of Nuclear Problems, Belarusian State University, **Minsk**, **Belarus**
• *11.2011; 11.2012; 09.2014; 10.2016.*	Visiting scientist, Institute of General and Inorganic Chemistry, Russian Academy of Sciences, **Moscow, Russia**
02.2012 – 12.2018	**Head of Laboratory, Institute of Solid State Physics at University of Latvia, Riga**

4. FELLOWSHIPS

1995-1997. Two Fellowships for six months; Centre for International Mobility (CIMO), Helsinki University of Technology, Espoo (**Finland**).

1997-1999. Two-year Senior Fellowship; Centre for Chemical Physics at University of Western Ontario, London (ON, **Canada**).

2005-2009. Five-year Fellowship for short-term visits (≤ four months annually) granted by National Science Foundation (USA); Materials Research Scientific and Engineering Center (MRSEC) at Northwestern University, Evanston (IL, **USA**).

5. INTERNATIONAL SCIENTIFIC EXPERTISE

2006-2014 EUROATOM-Latvia Fusion Project, in close collaboration with scientific groups from **Germany**, **Greece, Finland** and **Romania** (executive for "Materials Modeling" task in Latvian partner team);

2006-2010 EUROATOM ACTINET networking Project with **German** partners on Nuclear Fuels (participant).

2008-2011 EC Framework 7 Project on Nanoscale ICT Devices and Systems CATHERINE (Carbon nAnotube Technology for High-speed nExt-geneRation nanoInterconNEcts), in close collaboration with 10 partner scientific groups from **Italy, France, Netherlands, Sweden** and **Romania** (coordinator in charge for realization of Latvian partner team's part of scientific project as well as a member of Advisory Board for CATHERINE project);

2008-2011 EC Framework 7 Project on Advanced Nuclear Fuels *F*-BRIDGE (Basic Research for Innovative *F*uel Design for GEneration IV systems), in close collaboration with 6 partner scientific groups from **France**, **Germany**, and **Czech Republic** (participant);

2011-2014 FP 7 Marie Curie CACOMEL Project (Nano-carbon based components and materials for high frequency electronics), in collaboration with scientific groups from **Germany, Italy, Finland, Russia**, and **Belarus'** (coordinator of Latvian partner team);

Since 2015 EUROFUSION Project, in close collaboration with several scientific groups from **Germany**, **Estonia, Hungary, Spain** and **Sweden** (executive for "Enabling Research" and "WP Mat - Materials Modeling" tasks in Latvian partner teams);

Since 2016 ERA.Net RUS Plus Project WATERSPLIT devoted to simulations on photocatalytic abilities of semiconductor nanostructures, in close collaboration with scientific groups from **Germany** and **Russia** (coordinator of Project).

6. TEACHING EXPERIENCE

For several years (beginning with ***1975***), I had worked as a teacher of physics and mathematics in a few Secondary Schools of Riga. During my work at the Institute of Inorganic Chemistry, Latvian Academy of Science (1978-1994), I prepared and periodically gave a cycle of lectures on Computational Quantum Chemistry for young researchers (PhD and MS students) as well as for winners of Latvian Olympiads in Physics and Chemistry at Summer Schools organized in a number of Latvian peripheral cities and settlements (Mazsalaca, Kuldiga, etc.). I supervised several MS and PhD Theses. Beginning with ***2000*** a number of Masters of Science from the Transport and Telecommunication Institute, Riga, were trained by me for further PhD studentships at Osnabrück University and Max Planck Institute for Solid State Research, Stuttgart (both Germany), according to the programs of *ab initio* simulations on various advanced materials and processes. During several years, three of them successfully defended PhD Theses in Germany (S. Piskunov - 2003, D. Gryaznov - 2006, and Yu. Mastrikov - 2008). My PhD student D. Bocharov (involved in project EUROATOM ACTINET) successfully defended his Thesis at the University of Latvia in 2012 while my second PhD student A. Gopejenko (involved in EUROATOM-Latvia Fusion Project) completes his Thesis to be defended at the University of Latvia. My third PhD student A. Platonenko (involved in EUROFUSION Project, subproject WP Mat - Materials Modeling) has began his studentship since 2014.

7. LANGUAGE SKILLS: English, Russian (native), Latvian.

8. MAIN SCIENTIFIC ACTIVITIES

My scientific activities in ***80s years*** were mainly concerned with working out, testing and modifying of the computational code based on semi-empirical method of Complete Neglect of Differential Overlap, as parameterized by Boyd-Whitehead (*CNDO/BW*), simultaneously with calculations on various cluster models using this code. In particular, the chemisorption of H_2O molecules and their mono- and diatomic fragments on both clean and O-predosed densely packed faces of Al single-crystal as well as Al_n microclusters were simulated. *For the first time,* the mechanism of low-temperature dissociation of adsorbed water molecules was described, including formation of the molecular dimer as an intermediate stage of this process. The same semi-empirical *CNDO/BW* method was used later for qualitative simulations of possible structural transformations in the molecular crystal of yellow arsenic. The corresponding results were later verified using *ab initio* Hartree-Fock method, as implemented in *CRYSTAL-98* code.

The area of my scientific interests in ***90s*** was mainly concerned with the theoretical simulations on both regular and defective bulk and densely packed surfaces of metal oxides, including adsorption and adhesion processes on these substrates. The corresponding simulations on their periodic models were performed using calculations of the electronic properties and total energy surfaces based on both the first principles formalisms of Hartree-Fock (HF) method and Density Functional Theory (DFT), as implemented in consequently upgraded *ab initio CRYSTAL* code (*CRYSTAL-92*, *CRYSTAL-95* and *CRYSTAL-98*), as well as the semi-empirical *INDO* approach (Intermediate Neglect of Differential Overlap). Potentials and other parameters calculated by these methods were also used for further kinetic and thermodynamic simulations of the same processes, including metallic films growth on the metal oxide surfaces. DFT CO-LCGTF *CRYSTAL* calculations (where crystalline orbitals are constructed as linear combinations of Gaussian-type functions) were also performed on periodic models of pure Al (bulk and surface) as well as interfaces between densely-packed Al surfaces and oxygen molecules and atoms. *For the first time,* two possible mechanisms for the formation of Al_2O_3 nuclei during the initial stage of Al(111) surface oxidation were described.

Beginning with ***2000*** my scientific interests were focused on simulations of both regular and defective metal fluofires (LiF), oxides (α-Al_2O_3, $BaTiO_3$, Li_2O, MgO, $PbTiO_3$, $SrTiO_3$, TiO_2, ZnO), nitrides (AlN, BN, UN), *e.g.*,

their surfaces and interfaces with gases (O_2), metals (Ag, Cu, Ti) and salts (AgCl). For the corresponding *ab initio* calculations in parallel regime with total geometry optimization, there were used both new upgrades of *CRYSTAL* code (*CRYSTAL-03, CRYSTAL-06* and *CRYSTAL-09*) based on the formalism of localized Gaussian functions as well as a few upgrades of *VASP* code (Vienna *Ab initio* Simulation Package) based on the plane-wave techniques allowing atoms to relax into their instantaneous ground state. Since ***2005*** I have began nanostructure modeling and large-scale *ab initio* calculations (*e.g.,* carbon nanotubes and graphene nanoribbons, AlN NTs, BN NTs, TiO_2 and $SrTiO_3$ NTs), including simulation of their growth upon the metallic (Ni) catalyst as well as electrical and electronic properties of nanostructures and their junctions with various metallic substrates. Since ***2006*** I have been involved in theoretical simulation on growth of oxide dispersed particles (mainly Y_2O_3) inside Fe lattice (radiation-resistant steels) within the subproject "Materials Modeling" of EUROATOM.

Since ***2011*** I have began theoretical simulations and *ab initio* calculations of nanowires (beginning with rutile-based TiO_2 <001> and <110> NWs, then [001]-oriented cubic $SrTiO_3$ and [0001]-oriented hexagonal ZnO NWs) performing large-scale calculations using *CRYSTAL-09* and *CRYSTAL-14* codes. Within WP MAT subproject of EUROFUSION Project, I have studied stability and various properties of radiation-induced defects in corundum, using LCAO codes *CRYSTAL-14* for periodic supercell models and *NWChem* for cluster models. For WATERSPLIT Project, I have studied photocatalytic abilities of perfect semiconductor nanostructures ($SrTiO_3$, TiO_2 and ZnO NTs as well as NWs) of different morphologies and doped by C, N, S, Ag, Fe and other transition metals, using the same *CRYSTAL-14* and *NWChem* codes for calculations. I have also simulated core-shell ZnO-WS_2 NWs and WS_2 NTs.

9. PUBLICATIONS.

159 Journal and Proceeding papers as well as Book Chapters dealing with theoretical simulations. Citation – **1454**, Hirsch index - **21.**

10. LIST OF JOURNAL PAPERS AND BOOK CHAPTERS (THEORETICAL SIMULATIONS)

2016 ( )

159. **Yu.F. Zhukovskii**, A. Platonenko, S. Piskunov, and E.A. Kotomin, "*Ab initio* simulations on migration paths of interstitial oxygen in corundum". – *Nucl. Instr. Meth. Phys. Res. B*, **2016**, Vol. 374, N 1, p. 29–34.

158. O. Lisovski, A. Chesnokov, S. Piskunov, D. Bocharov, **Yu.F. Zhukovskii**, M. Wessel, and E. Spohr, "*Ab initio* calculations of doped TiO_2 anatase (101) nanotubes for photocatalytical water splitting applications". – *Mater. Sci. Semicond. Process.* **2016**, Vol. 42, N 1, p. 138-141.

157. **Yu.F. Zhukovskii**, S. Piskunov, O. Lisovski, A. Chesnokov, and D. Bocharov, "First principle evaluation of photocatalytic suitability for TiO_2-based nanotubes". – Chapter 4 in a book: *Semiconductor Photocatalysis - Materials, Mechanisms and Applications* (Ed. W. Cao, InTech Open Access Publisher, Rijeka, Croatia), **2016**, p. 105-133.

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156. 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**, Vol. 119, N 32, p. 18686−18696.

155. P.N. D'yachkov, V.A. Zaluev, S. Piskunov, and **Yu.F. Zhukovskii**, "Comparative analysis of the electronic structures of mono- and bi-atomic chains of IV, III–V and II–V group elements calculated using the DFT LCAO and LACW methods". - *Royal Soc. Chem. Advances*, **2015**, Vol. 5, N 111, p. 91751–91759.

154. A.V. Bandura, R.A. Evarestov, and **Yu.F. Zhukovskii**, "Energetic stability and photocatalytic activity of $SrTiO_3$ nanowires: *Ab initio* simulations". - *Royal Soc. Chem. Advances*, **2015**, Vol. 5, N 31, p. 24115-24125.

153. 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**, Vol. 90, N 9, 094013 (p. 1-7).

152. S. Bellucci, F. Micciulla, Yu.N. Shunin, **Yu.F. Zhukovskii**, V.I. Gopeyenko, N. Burlutskaya, T. Lobanova-Shunina, and A. Capobianchi, "Memory nanodevices based on carbon nanotube-Fe-Pt interconnects: Electromagnetic simulations and magnetically stimulated nanotube growth". - *J. Mater. Sci. Eng. B*, **2015**, Vol. 5, NN 3-4, p. 120-134.

151. Yu.N. Shunin, S. Bellucci, **Yu.F. Zhukovskii**, V.I. Gopejenko, N. Burlutskaya, T. Lobanova-Shunina, F. Micciulla, and A. Capobianchi, "Spintronic nanomemory and nanosensor devices based on carbon nanotube-Fe-Pt interconnects: Models and simulations". – Chapter in book: *Yu.N. Shunin, Spintronic Nanomemory and Nanosensor Devices* (Lambert Academic Publishing, Saarbrücken), **2015**, p. 2-49.

150. A. Platonenko, S. Piskunov, **Yu.F. Zhukovskii**, and E.A. Kotomin, "*Ab initio* simulations on Frenkel pairs of radiation defects in corundum". - *IOP Conf. Ser. Mater. Sci. Eng.*, **2015,** Vol. 77, 012001 (p. 1-5).

149. Yu.N. Shunin, **Yu.F. Zhukovskii**, V.I. Gopeyenko, N. Burlutskaya, T. Lobanova-Shunina, and S. Bellucci, "CNTs- and GNRs-based electromagnetic and spintronic devices: Models and simulations". - *Proc. Internat. Conf. „Physics, Chemistry and Application of Nanostructures"* (Nanomeeting-2015, Minsk, Belarus)*"* (Eds. V.E. Borisenko, S.V. Gaponenko, V.S. Gurin, and C.H. Kam; World Scientific, New Jersey, London, Singapore, Beijing, Shanghai, Hong Kong, Taipei, Chennai), **2015**, p. 207-210.

148. D. Fink, A. Kiv, Yu.N. Shunin, N. Mykytenko, T. Lobanova-Shunina, A. Mansharipova, T. Koycheva, R. Muhamediev, V. Gopeyenko, N. Burlutskaya, **Yu.F. Zhukovskii**, and S. Bellucci, "The nature of oscillations of ion currents in the ion track electronics". - *Comput. Model. & New Technol. (Latvia)*, **2015**, Vol. 19, N 6, p. 7-13.

147. Yu.N. Shunin, S. Bellucci, **Yu.F. Zhukovskii**, T. Lobanova-Shunina, N. Burlutskaya, and V.I. Gopeyenko, "Modelling and simulation of CNTs- and GNRs-based nanocomposites for nanosensor devices". - *Comput. Model. & New Technol. (Latvia)*, **2015**, Vol. 19, N 5A, p. 14-20.

146. Yu.N. Shunin, S. Bellucci, **Yu.F. Zhukovskii**, V.I. Gopeyenko, N. Burlutskaya, and T. Lobanova-Shunina, "Nanocarbon electromagnetics in CNT-, GNR- and aerogel-based nanodevices: models and simulations". - *Comput. Model. & New Technol. (Latvia)*, **2015**, Vol. 19, N 1A, p. 35-42.

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145. A.B. Usseinov, E.A. Kotomin, A.T. Akilbekov, **Yu F. Zhukovskii**, and J. Purans, "Hydrogen induced metallization of ZnO (1100) surface: *Ab initio* study". - *Thin Solid Films*, **2014**, Vol. 553, p. 38–42.

144. A.B. Usseinov, E.A. Kotomin, A.T. Akilbekov, **Yu.F. Zhukovskii**, and J. Purans, "Hydrogen adsorption on the ZnO ($1\bar{1}00$) surface: *Ab initio* hybrid density functional linear combination of atomic orbitals calculations". - *Phys. Scr.*, **2014**, Vol. 89, N 4, 045801 (p. 1-7).

143. Yu.N. Shunin, S. Bellucci, **Yu.F. Zhukovskii**, V.I. Gopejenko, N. Burlutskaya, T. Lobanova-Shunina, A. Capobianchi, and F. Micciulla, "CNT-Fe-Pt interconnect electromagnetic simulations for magnetically stimulated CNT growth and novel memory nanodevices". - *Comput. Model. & New Technol. (Latvia)*, **2014**, Vol. 18, N 1, p. 7-23.

142. **Yu.F. Zhukovskii**, "Boron and metal diborides". – Chapter 4 in book: *R.A. Evarestov, Theoretical Modeling of Inorganic Nanostructures* (Springer-Verlag, Berlin, Heidelberg), **2014**, p. 217-251.

141. **Yu.F. Zhukovskii**, "Group IV semiconductors". – Chapter 5 in book: *R.A. Evarestov, Theoretical Modeling of Inorganic Nanostructures* (Springer-Verlag, Berlin, Heidelberg), **2014**, p. 253-346.

140. **Yu.F. Zhukovskii**, "Nitrides of boron and group III metals". – Chapter 6 in book: *R.A. Evarestov, Theoretical Modeling of Inorganic Nanostructures* (Springer-Verlag, Berlin, Heidelberg), **2014**, p. 347-427.

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139. **Yu.F. Zhukovskii**, S. Piskunov, J. Kazerovskis, D.V. Makaev, and P.N. D'yachkov, "Comparative theoretical analysis of BN nanotubes doped with Al, P, Ga, As, In, and Sb". - *J. Phys. Chem. C*, **2013**, Vol. 117, N 27, p. 14235−14240.

138. J. Kazerovskis, S. Piskunov, **Yu.F. Zhukovskii**, P.N. D'yachkov, and S. Bellucci, "Formation of linear Ni nanochains inside carbon nanotubes: Prediction from density functional theory". - *Chem. Phys. Letters*, **2013**, Vol. 577, N 1, p. 92-95.

137. **Yu.F. Zhukovskii,** S. Piskunov, J. Begens, J. Kazerovskis, and O. Lisovski, "First-principles calculations of point defects in inorganic nanotubes (*Feature Article*)". - *phys. status solidi (b)*, **2013**, Vol. 250, N 4, p. 793-800.

136. 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**, Vol. 435, NN 1-3, p. 102–106.

135. R.A. Evarestov and **Yu.F. Zhukovskii**, "Four-faceted nanowires generated from densely-packed TiO_2 rutile surfaces: *Ab initio* calculations". - *Surf. Sci.*, **2013**, Vol. 608, NN 3-4, p. 226–240.

134. A. Usseinov, E.A. Kotomin, **Yu.F. Zhukovskii**, J. Purans, A. Sorokin, and A.T. Akilbekov, "Atomic and electronic structure of hydrogen on ZnO (1100) surface: *ab initio* hybrid calculations". - *IOP Conf. Series: Mater. Sci. Engineering*, **2013**, Vol. 49, 012054 (p. 1-4).

133. **Yu.F. Zhukovskii**, S. Piskunov, O. Lisovski, and J. Begens, "First principles simulations on doped TiO_2 and $SrTiO_3$ nanotubular photocatalysts for water-splitting hydrogen generation". - *Proc. Internat. Conf. „Physics, Chemistry and Application of Nanostructures* (Nanomeeting-2013, Minsk, Belarus)" (Eds. V.E. Borisenko, S.V. Gaponenko, V.S. Gurin, and C.H. Kam; World Scientific, New Jersey, London, Singapore), **2013**, p. 513-516.

132. S. Piskunov, J. Kazerovskis, **Yu.F. Zhukovskii**, P.N. Dyachkov, and S. Bellucci, "Incorporation of Ni nanofilament inside carbon nanotubes: DFT calculations". - *Proc. Internat. Conf. „Physics, Chemistry and Application of Nanostructures* (Nanomeeting-2013, Minsk, Belarus)" (Eds. V.E. Borisenko, S.V. Gaponenko, V.S. Gurin, and C.H. Kam; World Scientific, New Jersey, London, Singapore), **2013**, p. 139-142.

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131. **Yu.F. Zhukovskii**, S. Piskunov, and S. Bellucci, "Double-wall carbon nanotubes of different morphology: electronic structure simulations". - *Nanosci. Nanotechnol. Lett.*, **2012**, Vol. 4, N 11, p. 1074-1081.

130. Yu.N. Shunin, **Yu.F. Zhukovskii**, V.I. Gopeyenko, N. Burlutskaya, T. Lobanova-Shunina, and S. Bellucci, "Simulation of electromagnetic properties in carbon nanotubes and graphene-based nanostructures". - *J. Nanophoton.*, **2012**, Vol. 6, N 1, 061706 (p. 1-16)

129. 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**, Vol. 38, 012058 (p. 1-4)

128. O. Lisovski, S. Piskunov, **Yu.F. Zhukovskii**, and J. Ozolins, "*Ab initio* modeling of sulphur doped TiO_2 nanotubular photocatalyst for water-splitting hydrogen generation". - *IOP Conf. Series: Mater. Sci. Engineering*, **2012**, Vol. 38, 012057 (p. 1-5).

127. 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**, Vol. 38, 012015 (p. 1-4).

126. **Yu.F. Zhukovskii** and R.A. Evarestov, "*Ab initio* simulations on rutile-based titania nanowires". - *IOP Conf. Series: Mater. Sci. Engineering*, **2012**, Vol. 38, 012005 (p. 1-6).

125. R.A. Evarestov, D.B. Migas, and **Yu.F. Zhukovskii**, "Symmetry and stability of the rutile-based TiO_2 nanowires: models and comparative LCAO-plane wave DFT calculations". - *J. Phys. Chem. C*, **2012**, Vol. 116, N 24, p. 13395–13402.

124. Yu.N. Shunin, **Yu.F. Zhukovskii**, N. Burlutskaya, V.I. Gopeyenko, and S. Bellucci, "Simulation of fundamental properties of CNT- and GNR-metal interconnects for development of new nanosensor systems". - *Proc. NATO ARW „Nanodevices and Nanomaterials for Ecological Security"* (Eds. Yuri N. Shunin and Arnold E. Kiv; Springer: Dordrecht, **2012**), p. 237-262.

123. A. Gopejenko, **Yu.F. Zhukovskii**, P.V. Vladimirov, E.A. Kotomin, and A. Möslang, "Interaction between oxygen and yttrium impurity atoms as well as vacancies in *fcc* iron lattice: *Ab initio* modelling". - *Proc. NATO ARW „Nanodevices and Nanomaterials for Ecological Security"* (Eds. Yuri N. Shunin and Arnold E. Kiv; Springer: Dordrecht, **2012**), p. 149-160.

122. **Yu.F. Zhukovskii**, E.A. Kotomin, S. Piskunov, and S. Bellucci, "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.

121. Yu.N. Shunin**, Yu.F. Zhukovskii**, N. Burlutskaya, and S. Bellucci, "CNT-metal interconnects: Electronic structure calculations and resistivity simulations". - *J. Nanoelectronics & Optoelectronics*, **2012**, Vol. 7, N 1, p. 3–11.

120. **Yu.F. Zhukovskii**, D. Bocharov, D. Gryaznov, and E.A. Kotomin, "First principles simulations on surface properties and oxidation of nitride nuclear fuels". - Chapter 5 in book: *Advances in Nuclear Fuel* (Ed. Shripad T. Revankar, InTech Open Access Publisher, Rijeka, Croatia), **2012**, p. 95-122.

2011 (14)

119. R.A. Evarestov, **Yu.F. Zhukovskii**, A.V. Bandura, S. Piskunov, and M.V. Losev, "Symmetry and models of double-wall BN and TiO_2 nanotubes with hexagonal morphology". – *J. Phys. Chem. C*, **2011**, Vol. 115, N 29, p. 14067–14076.

118. D. Bocharov**,** D. Gryaznov**, Yu.F. Zhukovskii**, and E.A. Kotomin, "DFT calculations of point defects on UN(001) surface". **–** *Surf. Sci.*, **2011**, Vol. 605, NN 3-4, p. 396-400.

117. S. Piskunov, G. Zvejnieks, **Yu.F. Zhukovskii**, and S. Bellucci, "Atomic and electronic structure of both perfect and nanostructured Ni(111) surfaces: First-principles calculations". **–** *Thin Solid Films*, **2011**, Vol. 519, N 11, p. 3745–3751.

116. D. Bocharov, D. Gryaznov, **Yu.F. Zhukovskii**, and E.A. Kotomin, "*Ab initio* modeling of oxygen impurity atom incorporation into uranium mononitride surface and sub-surface vacancies". **–** *J. Nucl. Mater.*, **2011**, Vol. 416, NN 1-2, p. 200-204.

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80 papers were published in the most prestigious scientific journals with a high impact factor (IF > 1)

TITLE OF JOURNAL	NUMBER OF PUBLICATIONS	IF (2015)	TITLE OF JOURNAL	NUMBER OF PUBLICATIONS	IF (2015)
Phys. Rev. Letters	3	7.5	*J. Power Sources*	1	6.2
J. Phys. Chem. C	6	4.8	*Phys. Chem. Chem. Phys.*	1	4.5
Royal Soc. Chem. Advances	2	3.8	*Phys. Rev. B*	5	3.7
J. Comput. Chem.	1	3.6	*J. Phys. Chem. B*	1	3.3
Mater. Sci. Eng. C	2	3.1	*Int. J. Mol. Sci.*	1	2.9
Appl. Surf. Sci.	1	2.7	*J. Phys.: Cond. Matter*	5	2.4
Superlatt. Microstruct.	1	2.1	*Comput. Mater. Sci.*	4	2.1
Physica E	1	2.0	*Chem. Phys. Letters*	2	1.9
J. Nucl. Mater.	5	1.9	*J. Phys. Chem. Solids*	2	1.9
Solid State Commun.	2	1.9	*Surf. Sci.*	10	1.9
Vacuum	1	1.9	*Solid State Sci.*	1	1.8
Thin Solid Films	2	1.8	*J. Nanophoton.*	1	1.7
J. Mol. Struct.	2	1.6	*phys. status solidi (b)*	4	1.5
Eur. Phys. J. B	1	1.4	*Int. J. Quant. Chem*	2	1.4
THEOCHEM	1	1.4	*Microelectronic Eng.*	1	1.2
Nucl. Instr. Meth. B	6	1.1	*Phys. Scripta*	2	1.1

11. PARTICIPATION AT INTERNATIONAL CONFERENCES.

290 oral (*e.g.*, plenary and invited) and poster presentations dealing with the quantum chemistry and other theoretical simulations were prepared for **145** international conferences, meetings, seminars and symposiums (including **265** abstracts published for them) organized in **28** countries (*Austria, Belarus, Canada, Czech Rep., Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Italy, Kazakhstan, Latvia, Lithuania, Netherlands, Poland, Romania, Russia, Slovenia, Spain, Sweden, Switzerland, Tajikistan, UK, Ukraine, USA, Uzbekistan*).

12. CONFERENCE PRESENTATIONS DEALING WITH THEORETICAL SIMULATIONS

2016

5th International Workshop on Nanocarbon Photonics and Optoelectronics (Lappeenranta, *Finland*, August, 2016),

290. Yu.N. Shunin, D. Fink, A.E. Kiv, L. Alfonta, A. Mansharipova, R. Muhamediyev, **Yu.F. Zhukovskii**, T. Lobanova-Shunina, N. Burlutskaya, V.I. Gopeyenko, and S. Bellucci, "Theory and modelling of physical and bio-nanosensor systems". – Abstract: p. 101.

19th International Conference on Defects in Insulating Materials, ICDIM'16 (Lyon, *France*, July, 2016).

289. R.A. Evarestov, **Yu.F. Zhukovskii**, S. Piskunov, A. Platonenko, E.A. Kotomin, and J. Maier, "*Ab initio* simulations of interstitial oxygen in corundum". – Abstract: Mo-O-15.

College on Multiscale Computational Modeling of Materials for Energy Applications (Trieste, *Italy*, July 2016).

288. O. Lisovski, S. Piskunov, **Yu.F. Zhukovskii**, and E. Spohr, "DFT modeling of doped ZnO nanowires with various diameters".

E-MRS 2016 Spring Meeting (Lille, *France*, May, 2016).

287. R.I. Eglitis, S. Piskunov, and **Yu.F. Zhukovskii**, "*Ab initio* calculations of $SrZrO_3$ bulk and surface *F* centers as well as $BaTiO_3/SrTiO_3$, $SrZrO_3/PbZrO_3$, and $SrTiO_3/PbTiO_3$ heterostructures". – Abstract: BB.8.3.

286. Yu.A. Mastrikov, P.V. Vladimirov, V.A. Borodin, A. Gopejenko, **Yu.F. Zhukovskii**, E. A. Kotomin, and A. Möslang, "Ab initio modelling of *n*Y/*m*O nanoclusters in *bcc* Fe lattice". – Abstract: BB.9.2.

285. **Yu.F. Zhukovskii**, O. Lisovski, S. Piskunov, and R.A. Evarestov, "Quantum chemical simulations of doped ZnO nanowires for photocatalytic hydrogen generation". – Abstract: BB.13.2.

284. A. Platonenko, **Yu.F. Zhukovskii**, S. Piskunov, and E.A. Kotomin, "*Ab initio* simulations of radiation-induced oxygen defects in corundum". – Abstract: BB.P1.8.

*14th International Conference "Information Technologies and Management", IT&M'2016 (*Riga, *Latvia*, April, 2016).

283. Yu.N. Shunin, L. Alfonta, D. Fink, A.E. Kiv, A. Mansharipova, R. Muhamediyev, **Yu.F. Zhukovskii**, and T. Lobanova-Shunina, "Modelling and simulation of electric response of nanocarbon nanocomposites and nanoporous polymer based structures for nanosensor devices". Abstract: p. 11-14.

282. M. Sokolov, Yu.A. Mastrikov, A. Gopejenko, **Yu.F. Zhukovskii**, and E.A. Kotomin, "Ab initio modelling of Y-O complexes in α-Fe matrix". Abstract: p. 18-19.

281. **Yu.F. Zhukovskii**, O. Lisovski, S. Piskunov, and R.A. Evarestov, "Suitability of doped [0001]-oriented ZnO nanowires of different sizes for photocatalytic applications: DFT-LCAO simulations". Abstract: p. 20-21.

280. A. Gopejenko, **Yu.F. Zhukovskii**, S. Piskunov, and E.A. Kotomin, "First principle calculations of PZT varying Zr and Ti concentrations". Abstract: p. 22.

279. A. Platonenko, **Yu.F. Zhukovskii**, S. Piskunov, and E.A. Kotomin, "*Ab initio* calculations of charged point defects in corundum". Abstract: p. 23.

50th Russian School on Condensed State Physics (St. Petersburg, *Russia*, March, 2016).

278. D. Bocharov, **Yu.F. Zhukovskii**, S. Piskunov, O. Lisovski, and A. Chesnokov, "First principles evaluation of photocatalytic suitability for TiO2-based nanotubes". Abstract: p. 214.

32th ISSP Conference (Riga, *Latvia*, February, 2016).

277. M. Sokolov, Yu.A. Mastrikov, A. Gopejenko, **Yu.F. Zhukiovskii**, and E.A. Kotomin,"*Ab initio* modelling of Y-O complexes in α-Fe matrix". – Abstract: p. 97.

276. A. Gopejenko, **Yu.F. Zhukovskii**, S. Piskunov, E.A. Kotomin, "Variation of Zr and Ti concentration in PZT: first principles calculations on the electronic structure". – Abstract: p. 95.

275. A. Platonenko, **Yu.F. Zhukovskii**, S. Piskunov, and E.A. Kotomin, "First principles calculations of interstitial oxygen atom migration paths in corundum". – Abstract: p. 94.

274. A. Gopejenko, **Yu.F. Zhukovskii**, P.V. Vladimirov, E.A. Kotomin, Yu.A. Mastrikov, V.A. Borodin, and A. Möslang, "*Ab initio* calculations of O and V_{Fe} interaction in fcc Fe lattice". – Abstract: p. 37.

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11th International Conference "Functional Materials and Nanotechnologies" FM&NT-2015 (Vilnius, *Lithuania*, October, 2015).

273. Yu.N. Shunin, S. Bellucci, **Yu.F. Zhukovskii**, T. Lobanova-Shunina, N Burlutskaya, and V.I. Gopeyenko, "Modeling and simulation of CNTs- and GNRs-based nanocomposites for nanosensor devices". Abstract: p. 45.

EuroNanoForum-2015 (Riga, *Latvia*, June, 2015).

272. A.V. Bandura, R.A. Evarestov, and **Yu.F. Zhukovskii**, "Comparative analysis of four-faceted [001]-oriented nanowires formed from TiO_2 rutile and $SrTiO_3$ cubic phases: *Ab initio* simulations".

271. A. Chesnokov, O. Lisovski. S. Piskunov, D. Bocharov, and **Yu.F. Zhukovskii**, "Photocatalytic properties of doped TiO_2 nanotubes: Prediction from first principles".

270. Yu.N. Shunin, V.I. Gopeyenko, N. Burlutskaya, T. Lobanova-Shunina, S. Bellucci, and **Yu.F. Zhukovskii**, "Electromechanical properties of carbon-based nanocomposites for pressure and temperature nanosensors".

International Conference NANOMEETING-2015 (Minsk, *Belarus,* May, 2015).

269. Yu.N. Shunin, **Yu.F. Zhukovskii**, V.I. Gopeyenko, N. Burlutskaya, T. Lobanova-Shunina, and S. Bellucci, "CNTs- and GNRs-based electromagnetic and spintronic devices: Models and simulations". – Abstract: p. 207.

Spring European Materials Research Society (EMRS) Meeting (Lille, France, May, 2015).

268. A. Chesnokov, O. Lisovski, D. Bocharov, S. Piskunov, and **Yu.F. Zhukovskii**, "*Ab initio* simulations on pristine and doped TiO2 anatase (101) nanotubes". – Abstract: B/P1.7.

267. **Yu.F. Zhukovskii**, A. Platonenko, S. Piskunov, and E.A. Kotomin, "*Ab initio* computer simulations of radiation defects in corundum". – Abstract: G.2.2.

266. Yu.A. Mastrikov, P.V. Vladimirov, V.A. Borodin, A. Gopejenko, **Yu.F. Zhukovskii**, E.A. Kotomin, and A. Möslang, "Interaction of yttrium and oxygen with vacancy clusters within bcc-Fe matrix". – Abstract: G/P.11.

265. A. Usseinov, E.A. Kotomin, A.T. Akilbekov, **Yu.F. Zhukovskii**, J. Purans, and F. Abuova, "Hydrogen migration and stability in ZnO: *Ab initio* calculations". – Abstract: N/P2.27.

13th International Conference "Information Technologies and Management", IT&M'2015 (Riga, *Latvia*, April, 2015).

264. Yu.N. Shunin, D. Fink, S. Bellucci, A.E. Kiv, T. Lobanova-Shunina, **Yu.F. Zhukovskii**, and V.I. Gopeyenko, "Nanotechnology and health nanodiagnostic tools". – Abstract: p. 15-17.

263. Yu.N. Shunin, S. Bellucci, T. Lobanova-Shunina, **Yu.F. Zhukovskii**, N. Burlutskaya, and V.I. Gopeyenko,"Models and simulations of CNTs- and GNRs-based electromagnetic and spintronic devices". – Abstract: p. 18-20.

262. A. Gopejenko, **Yu.F. Zhukovskii**, P.V. Vladimirov, V.A. Borodin, E.A. Kotomin, Yu.A. Mastrikov, and A. Möslang, "*Ab initio* calculations of Y, O and V_{Fe} migration barriers inside *fcc*-Fe lattice". – Abstract: p. 21.

261. **Yu.F. Zhukovskii**, R.A. Evarestov, and A.V. Bandura, "Photocatalytic efficiency of SrTiO3 nanowires: ab initio modeling". – Abstract: p. 22-23.

260. A. Chesnokov, O. Lisovski, D. Bocharov, S. Piskunov, and **Yu.F. Zhukovskii**, "Correlation between morphology of TiO_2 nanotubes and their photocatalytic abilities: *ab initio* study". – Abstract: p. 28-29.

259. A. Platonenko, **Yu.F. Zhukovskii**, S. Piskunov, and E.A. Kotomin, "*Ab initio* simulations on interstitial oxygen atom in corundum". – Abstract: p. 31.

49th Russian School on Condensed State Physics (St. Petersburg, *Russia,* March, 2015).

258. A. Platonenko, S. Piskunov, **Yu.F. Zhukovskii**, and E.A. Kotomin, "*Ab initio* simulation of point defects and Frenkel pairs in corundum crystal (Russ.)". – Abstract: p. 168

31th ISSP Conference (Riga, *Latvia,* February, 2015).

257. A. Platonenko, S. Piskunov, **Yu.F. Zhukovskii**, and E.A. Kotomin, "*Ab initio* simulations on neutral point defects and Frenkel pairs in corundum (Latv.)". Abstract: p. 40.

256. A. Gopejenko, **Yu.F. Zhukovskii**, P.V. Vladimirov, E.A. Kotomin, Yu.A. Mastrikov, V.A. Borodin, and A. Möslang, "*Ab initio* calculations of Y, O and V_{Fe} diffusion barriers inside *fcc*-Fe lattice (Latv.)". – Abstract: p. 41.

255. A. Chesnokov, O. Lisovski, D. Bocharov, S. Piskunov, and **Yu.F. Zhukovskii**, "Connection between electronic structure of TiO_2 nanotubes and their morphology: *Ab initio* study (Latv.)". – Abstract: p. 42.

2014 (20)

15th International Workshop on Nanoscience and Nanotechnology, n&n-2014 (Frascati, *Italy,* October, 2014).

254. Yu.N. Shunin, S. Bellucci, **Yu.F. Zhukovskii**, V.I. Gopeyenko, T. Lobanova-Shunina, and N. Burlutskaya, "Nanocarbon-based Fe-Pt spintronic devices: models and simulation".

Joint 12th RCBJCF Symposium and 10th FMNT Conference (Riga, *Latvia,* September-October, 2014).

253. **Yu.F. Zhukovskii**, R.A. Evarestov, and A.V. Bandura, "First principles simulations on stoichiometric $SrTiO_3$ nanowires'. – Abstracts: p. 160.

252. Yu.N. Shunin, **Yu.F. Zhukovskii**, V.I. Gopeyenko, N. Burlutskaya, T. Lobanova-Shunina, and S. Bellucci, "Electromechanics and electromagnetics of CNT- and graphene-based nanoporous materials: Interconnects and nanosensoring". – Abstracts: p. 264.

251. A. Chesnokov, O. Lisovskii, 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". – Abstracts: p. 272.

250. A. Usseinov, E.A. Kotomin, **Yu.F. Zhukovskii**, J. Purans, A.T. Akilbekov, and A.K. Dauletbekova, "Electronic effects on hydrogen-adsorbed surfaces of ZnO: First principles study". – Abstracts: p. 275.

249. A. Platonenko, S. Piskunov, **Yu.F. Zhukovskii**, and E.A. Kotomin, "*Ab initio* simulations on Frenkel pairs of radiation defects in corundum". – Abstracts: p. 278.

248. A. Gopejenko, **Yu.F. Zhukovskii**, P.V. Vladimirov, E.A. Kotomin, Yu.A. Mastrikov, V.A. Borodin, and A. Möslang, "*Ab initio* calculations of interactions between Y and O impurity atoms and vacancies in *bcc*- and *fcc*-iron lattices". – Abstract: p. 282.

Fall European Materials Research Society (EMRS) Meeting (Warsaw, *Poland,* September, 2014).

247. D. Gryaznov, D. Bocharov, E.A. Kotomin, and **Yu.F Zhukovskii**, "*Ab initio* simulations of oxygen interaction with surfaces and interfaces in uranium mononitride". – Abstract: G9.44.

4th International Workshop on Nanocarbon Photonics and Optoelectronics (Polvijarvi, *Finland*, July-August, 2014).

246. Yu.N. Shunin, **Yu.F. Zhukovskii**, V.I. Gopeyenko, N. Burlutskaya, T. Lobanova-Shunina, and S. Bellucci, "Simulation of electromagnetic properties in CNT- and graphene-based nanomaterials and nanodevices". – Abstract: p. 74.

Spring European Materials Research Society (EMRS) Meeting (Lille, *France,* May, 2014).

245. **Yu.F. Zhukovskii**, S. Piskunov, O. Lisovskii, J. Begens, and E. Spohr, „Doped TiO_2 and $SrTiO_3$ nanotubes for photocatalytic applications: Predictions from first principles". – Abstract: EO.8.2.

244. Yu.A. Mastrikov, P.V. Vladimirov, V.A. Borodin, A. Gopejenko, **Yu.F. Zhukovskii**, E.A. Kotomin, and A. Möslang, „*Ab initio* simulation of the initial steps of the ODS particle formation process in *bcc* iron matrix". – Abstract: EP.2.73.

12th International Conference "Information Technologies and Management", IT&M'2014 (Riga, *Latvia*, April, 2014).

243. Yu.N. Shunin, **Yu.F. Zhukovskii**, V.I. Gopeyenko, N. Burlutskaya, T. Lobanova-Shunina, and S. Bellucci, "Simulation of fundamental properties in CNT- and graphene-based nanoporous materials: Electromechanics and Electromagnetics". Abstracts: p. 17-18.

242. **Yu.F. Zhukovskii**, S. Piskunov, A. Platonenko, and E.A. Kotomin, "Simulation of radiation-induced Frenkel pairs in α-Al_2O_3: Optimization of computational procedure". Abstracts: p. 19-20.

241. A. Gopejenko, **Yu.F. Zhukovskii**, P.V. Vladimirov, Yu.A. Mastrikov, E.A. Kotomin, V.A. Borodin, and A. Möslang, "*Ab initio* calculations of interactions between Y, O impurity atoms and Fe vacancies for ODS steel implementation in fusion reactors". Abstracts: p. 21-22.

240. A. Platonenko, S. Piskunov, D. Bocharov, **Yu.F. Zhukovskii**, and S. Bellucci, "First principles simulations on Fe-Pt nanoclusters of various morphology and CNT growth upon them". Abstracts: p. 23-25.

239. A. Chesnokov, O. Lisovski, D. Bocharov, S. Piskunov, **Yu.F. Zhukovskii**, M. Wessel, and E. Spohr, "Quantum-chemical study of pristine and doped TiO_2 nanotubes for water photocatalysis". Abstracts: p. 26-28.

48th Russian School on Condensed State Physics (St. Petersburg, *Russia*, March, 2014).

238. D. Bocharov, S. Piskunov, O. Lisovski, **Yu.F. Zhukovskii**, and E. Spohr, "Quantum chemical simulations of TiO_2 nanotubes for photocatalytical water splitting (Russ.)". - Abstract: p. 166.
30th ISSP Conference (Riga, *Latvia*, February, 2014).

237. A. Platonenko, S. Piskunov, **Yu.F. Zhukovskii**, and D. Bocharov, "Fe-Pt nanoparticle structure: *Ab initio* calculations (Latv.)". - Abstracts: p. 33.

236. J. Begens, S. Piskunov, **Yu.F. Zhukovskii**, and O. Lisovski, "Simulations and comparison of doped $SrTiO_3$ and TiO_2 nanotubes for application in photocatalytic water separation (Latv.)". - Abstracts: p. 35.

235. A. Gopejenko, **Yu.F. Zhukovskii**, P.V. Vladimirov, E.A. Kotomin, Yu.A. Mastrikov, V.A. Borodin, and A. Möslang, "First principles calculations of the energy barriers for different trajectories of Y atom migration inside fcc-Fe lattice (Latv.)". - Abstracts: p. 36.

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6th International Conference on Innovative Information Technologies, IIT-2013 (Vilnius, *Lithuania*, November, 2013).

234. Yu.N. Shunin, **Yu.F. Zhukovskii**, V.I. Gopeyenko, T. Lobanova-Shunina, N. Burlutskaya, and S. Bellucci, "Carbon based nanosensor systems for intelligent systems: Modeling and technology."

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128. R.A. Evarestov and **Yu.F. Zhukovskii**, "Symmetry of inorganic nanotubes: from bulk crystal space group to monolayer diperiodic group and nanotube line group". – Abstract: p. 38.

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127. Yu.N. Shunin, **Yu.F. Zhukovskii**, V.I. Gopeyenko, and N. Shunina, "Theoretical simulations of nanoelectronic devices: quantum dots, nanowires and carbon nanotubes". – Abstract: p. 98-99.

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124. Yu.N. Shunin, **Yu.F. Zhukovskii**, and S. Bellucci, "Theoretical simulations on conductivity and resistivity of carbon nanotubes and CNT-Ni interconnects using effective media approach". – Abstract: p. 115.

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123. D. Bocharov, D. Gryaznov, **Yu.F. Zhukovskii**, and E.A. Kotomin, "*Ab initio* calculations on the atomic and electronic structure of defective UN(001) surface". – Abstract: p. 32-33.

122. A. Gopejenko, **Yu.F. Zhukovskii**, P.V. Vladimirov, E.A. Kotomin, and A. Möslang, "Simulation of yttrium oxide particle formation in iron in support of ODS steel development". – Abstract: p. 30-31.

121. Yu.N. Shunin, **Yu.F. Zhukovskii**, and S. Bellucci, "Theoretical simulations of carbon nanotubes devices". – Abstract: p. 17-18.

120. **Yu.F. Zhukovskii**, S. Piskunov, E.A. Kotomin, and S. Bellucci, "Carbon nanotubes in project CATHERINE: 2D periodic model of CNT bundle growth on the nanostructured Ni(111) surface: *ab initio* simulations". – Abstract: p. 15-16.

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119. A. Gopejenko, **Yu.F. Zhukovskii**, P. Vladimirov, E.A. Kotomin, and A. Moslang, "Simulations on solution of yttrium and oxygen atoms in *fcc* iron lattice". – Abstract: p. 101.

118. D. Bocharov, D. Gryaznov, **Yu.F. Zhukovskii**, and E.A. Kotomin, "Perfect and defective (001) surface of uranium nitride: *ab initio* calculations". – Abstract: p. 100.

117. **Yu.F. Zhukovskii**, V. Kashcheyevs, S. Piskunov, Yu.N. Shunin, and E.A. Kotomin, "Participation of ISSP group in the EC FP7 project: carbon nanotube technology for high-speed next-generation nano-interconnects (*CATHERINE*) ". – Abstract: p. 89.

116. Yu. Shunin, **Yu.F. Zhukovskii**, and S. Bellucci, "*Ab initio* calculations of electronic properties and conductivity of carbon nanotubes and CNT-Ni interconnects in the effective media approach". – Abstract: p. 72.

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114. D. Bocharov, **Yu.F. Zhukovskii**, and E.A. Kotomin, "Chemisorption of a molecular oxygen on the UN (001) surface (Latv.)". Abstract: p. 54.

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113. **Yu.F. Zhukovskii**, S. Piskunov, E.A. Kotomin, and D.E. Ellis, "Comparison of the atomic and electronic structure of single *F*-centers in cubic $PbZrO_3$, $PbTiO_3$, and $SrTiO_3$ perovskites". – Abstract: C.9.1.

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112. **Yu.F. Zhukovskii**, S. Piskunov, E.A. Kotomin, and S. Bellucci. "2D periodic models of Ni(111)/CNT interconnects (bundles): *ab initio* calculations". – Abstract: p. 35-37.

111. Yu.N. Shunin, **Yu.F. Zhukovskii**, and S. Bellucci, "Simulations of properties of CNT/Ni(111) interconnects using the effective media approach". – Abstract: p. 32-34.

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110. E.A. Kotomin, **Yu.F. Zhukovskii**, and J. Maier, "Atomistic modelling of a new mechanism for a Li storage in batteries". – Abstract: A61, p.13.

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107. **Yu.F. Zhukovskii**, Yu.N. Shunin, S. Piskunov, and E.A. Kotomin, "First principles simulations of interconnects between CNTs and Ni(111) film". – Abstract: p. 284.

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104. 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". – Abstract: I-7.

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102. A. Gopeyenko, **Yu.F. Zhukovskii**, P.V. Vladimirov, and E.A. Kotomin, "*Ab initio* Calculations of oxygen and yttrium impurities in *fcc* Fe". – Abstract: p. 23.

101. D. Bocharov, **Yu.F. Zhukovskii**, and E.A. Kotomin, "Spontaneous dissociation of O_2 molecules at oxygen adsorption on the UN(001) surface". – Abstract: p. 14.

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100. Yu.N. Shunin, S. Piskunov, **Yu.F. Zhukovskii**, and E.A. Kotomin, "Modelling of fundamental properties for interconnects between Ni film and carbon nanotubes". – Abstract: p. 167.

99. D. Bocharov, **Yu.F. Zhukovskii**, R.A. Evarestov, E.A. Kotomin, and A. Bandura, "Atomic and molecular oxygen adsorption on the UN (001) surface". – Abstract: p. 87.

98. **Yu.F. Zhukovskii**, S. Piskunov, B. Berzina, L. Trinkler, and S. Bellucci, "Atomic and electronic structure of single-walled BN nanotubes containing nitrogen vacancies". – Abstract: p. 25.

97. E.A. Kotomin, Yu.A. Mastrikov, **Yu.F. Zhukovskii**, S. Piskunov, and J. Maier, "First-principles modelling of perovskite surface reactivity". – Abstract: p. 19.

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96. D. Bocharov, **Yu.F. Zhukovskii**, D. Gryaznov, R.A. Evarestov, and E.A. Kotomin, "Structure and properties of UN nuclear fuels: quantum chemistry approach (Latv.)". – Abstract: p. 6.

95. A. Gopejenko, **Yu.F. Zhukovskii**, P.V. Vladimirov, and E.A. Kotomin, "*Ab initio* calculations of O and Y impurities in Fe *fcc* lattice (Latv.)". Abstracts: p. 4.

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94. P.V. Vladimirov, V.A. Borodin, A. Möslang, A.I. Ryazanov, E.A. Kotomin, and **Yu.F. Zhukovskii**, "Modeling of yttrium oxide particle precipitation in iron". – Abstract: p. 371.

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92. **Yu.F. Zhukovskii**, S. Piskunov, B. Berzina, L. Trinkler, and S. Bellucci, "*Ab initio* simulations on the atomic and electronic structure of single-walled BN nanotubes and nanoarches". – Abstract: p. 38-39.

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91. **Yu.F. Zhukovskii**, E.A. Kotomin, P. Balaya, J. Maier, "Enhanced interfacial lithium storage in nanocomposites of transition metals with LiF or Li_2O: experimental studies and theoretical simulations". – Abstract: p. 58.

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87. **Yu.F. Zhukovskii**, A.I. Popov, C. Balasubramanian, and S. Belucci, "Theoretical simulations of regular and defective aluminum nitride nanotubes". – Abstract: p. 53.

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86. D. Bocharov, **Yu.F. Zhukovskii**, and E.A. Kotomin, "First-principles simulations of oxygen adsorption on perfect and defective UN(001) surface (Latv.)". – Abstract: p. 17.

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83. **Yu.F. Zhukovskii**, E.A. Kotomin, R.A. Evarestov, and D.E. Ellis, "Periodic quantum chemical simulations of point defects in metal oxides". – Abstract: p. 116.

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82. D. Fuks, E.A. Kotomin, **Yu.F. Zhukovskii**, and D. Ellis, "Coin metal adsorption on perfect and defective MgO (001) surfaces". Abstract: p.27.

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80. D. Fuks, **Yu.F. Zhukovskii**, E.A. Kotomin, and D.E. Ellis, "Role of surface *F*-centers in formation of ultra-thin Ag and Cu films on the MgO(001) substrate". Abstracts: P14.

79. **Yu.F. Zhukovskii**, S. Piskunov, E.A. Kotomin, E. Heifets, and D.E. Ellis, "A comparative study of cubic $PbZrO_3$ and $SrTiO_3$ perovskites containing single *F*-centers: *ab initio* simulations". Abstracts: P13.

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77. **Yu.F. Zhukovskii**, D. Fuks, E.A. Kotomin, and D.E. Ellis, "Difference of metal film growth modes on perfect and defective MgO surface". – Abstract: p. 109.

76. **Yu.F. Zhukovskii**, E.A. Kotomin, Yu.A. Mastrikov, S. Piskunov, K.L. Tsemekhman, and D.E. Ellis, "*Ab initio* simulations of isolated *F* centers in cubic $SrTiO_3$ perovskite". – Abstract: p. 42.

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75. **Yu.F. Zhukovskii** and E.A. Kotomin, "Theoretical simulation on the enhanced Li storage in the interfaces between transition metals and ionic lithium compounds used in Li batteries". – Abstract: p. 83.

74. E.A. Kotomin, **Yu.F. Zhukovskii**, and Yu.A. Mastrikov, "First-principles modeling of surfaces and reactivity of oxide and ABO_3 perovskite surfaces". – Abstract: p. 33.

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72. **Yu.F. Zhukovskii**, A.I. Popov, C. Balasubramanian, and S. Bellucci, "Structural and electronic properties of single-walled AlN nanotubes of different chiralities and sizes". – Abstract: p. 71.

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71. **Yu.F. Zhukovskii**, E.A. Kotomin, P. Balaya, and J. Maier, "First principles modelling of interfacial Li storage". – Abstract: p. 473.

70. **Yu.F. Zhukovskii**, E.A. Kotomin, Yu.A. Mastrikov, and J. Maier, "*Ab initio* study of ionic conductivity on AgCl/α-Al_2O_3(0001) interface". – Abstract: p. 472.

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69. S. Krischok, P. Stracke, O. Höfft, and V. Kempter, **Yu.F. Zhukovskii**, and E.A. Kotomin, "Cu(Pd) atom interaction with ultrathin MgO films on W(110): first principles calculations and electron (MIES and UPS) spectroscopy". – Abstract: p. 191-192.

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67. D. Fuks, **Yu.F. Zhukovskii**, E.A. Kotomin, and D.E. Ellis, "Coin metal adsorbtion on perfect and defective MgO(001) surfaces: the electronic structure calculations and film growth thermodynamics". – Abstract: p. 227.

66. **Yu.F. Zhukovskii**, E.A. Kotomin, and D. Ellis, "First principles simulation on the defect-free Cu/$BaTiO_3$(001) cubic interfaces". – Abstract: p. 155.

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65. P. Balaya, **Yu.F. Zhukovskii**, M. Dolle, E.A. Kotomin, H. Li, and J. Maier, "Experimental and theoretical evidence for novel interfacial mechanism for lithium storage in nanocomposites". – Abstract: p. 164.

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64. P. Balaya, M. Dolle, H. Li, Y. Hu, J. Jamnik, **Yu.F. Zhukovskii**, E.A. Kotomin, and J. Maier, "Nanocrystallinity effects in lithium battery electrodes with RuO_2 as a model material". – Abstract: p. 72-73.

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63. R.A. Evarestov, E.A. Kotomin, and **Yu.F. Zhukovskii**, "DFT study of a single *F* center in cubic $SrTiO_3$ perovskite: periodic model of aperiodic system". – Abstract: p. 26.

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60. **Yu.F. Zhukovskii**, S. Piskunov, E.A. Kotomin, O. Sychev, and G. Borstel, "DFT modeling of copper adhesion on regular $BaTiO_3$(001) surfaces". – Abstract: p. 196.

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59. **Yu.F. Zhukovskii** and E.A. Kotomin, "Transition metal adsorption on defective MgO(001) surface: *ab initio* study (Engl.)". – Abstract: p. 71.

58. F. Illas, N. Lopez, J. Carrasco, E.A. Kotomin, **Yu.F. Zhukovskii**, S. Piskunov, J. Maier, and K. Hermansson, "First principles simulations of *F* center in $SrTiO_3$ perovskite". – Abstract: p. 50.

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57. D. Fuks, S. Dorfman, **Yu.F. Zhukovskii**, E.A. Kotomin, and A.M. Stoneham, "Theory of the growth mode for a thin metallic film on an insulating substrate". – Abstract: SS3-ThM10.

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55. **Yu.F. Zhukovskii**, E.A. Kotomin, Yu.A. Mastrikov, and J. Maier, "*Ab initio* simulations on AgCl(111) surface and AgCl(111)/α-Al_2O_3(0001) interface". – Abstract: H/P.26.

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53. Yu.A. Mastrikov, **Yu.F. Zhukovskii**, E.A. Kotomin, and Yu.N. Shunin, "Diffusion of silver ions on the AgCl(111)/α-Al_2O_3(0001) interface: first principles simulation". – Abstract: p. 25-26.

52. **Yu.F. Zhukovskii**, O. Sychev, E.A. Kotomin, G. Borstel, and Yu.N. Shunin, "DFT modeling of transition metal adhesion on the MgO(001) surface". – Abstract: p. 23-24.

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51. **Yu.F. Zhukovskii** and E.A. Kotomin, "Influence of defects on the adhesion of transition metals on non-polar MgO(001) surface: comparative theoretical analysis (Latv.)". – Abstract: p. 47.

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48. **Yu.F. Zhukovskii**, E.A. Kotomin, and G. Borstel, "Comparative analysis of copper and silver adhesion on the MgO substrate". – Abstract: p. 64.

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47. **Yu.F. Zhukovskii**, E.A. Kotomin, D. Fuks, and S. Dorfman, "First principles simulations of the regular Cu/MgO(001) interface". – Abstract: 17104 (p. 1-2).

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46. **Yu.F. Zhukovskii**, E.A. Kotomin, D. Fuks, S. Dorfman, A.M. Stoneham, O. Sychev, and G. Borstel, "First-principles simulations of 2D Cu/MgO(001) superlattices". – Abstract: F-VI.3.

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44. Yu.N. Shunin, K. Budilov, **Yu.F. Zhukovskii**, O. Sychev, and G. Borstel, "Electronic and elastic properties of Cu-interconnects". – Abstract: p. 18-19.

43. Yu.A. Mastrikov, **Yu.F. Zhukovskii**, E.A. Kotomin, and Yu.N. Shunin, "Hartree-Fock simulations on the AgCl(111)/α–Al_2O_3(0001) interface ". – Abstract: p. 14-15.

42. O. Sychev, **Yu.F. Zhukovskii**, E.A. Kotomin, G. Borstel, and Yu.N. Shunin, "DFT simulations of the Cu/MgO(001) interface". – Abstract: p. 12-13.

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40. **Yu.F. Zhukovskii, "**On the mechanism of initial stage of metal adhesion on ceramic surface". – Abstract: p. 27.

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39. **Yu.F. Zhukovskii**, E.A. Kotomin, and P.W.M. Jacobs, "Large-scale computer simulations of metal-oxide interfaces with defects". – Abstract: p. 38.

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38. D. Fuks, S. Dorfman, **Yu.F. Zhukovskii**, E.A. Kotomin, and A.M. Stoneham, "Thermodynamics of the initial state of growth for a thin metallic film on an insulating substrate". – Abstract: p. 58.

37. E.A. Kotomin, J. Maier, A.M. Stoneham, **Yu.F. Zhukovskii**, D. Fuks, and S. Dorfman, "*Ab initio* modeling of metal adhesion to ceramics". – Abstract: p. 56.

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