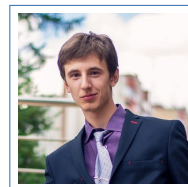


Anton Boev

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Personal Information

Date of Birth February 27, 1994

Sex Male

Citizenship Russia

Languages English (upper-intermediate), Russian (native speaker)

Academic degree Candidate of Sciences in Physics and Mathematics (2019)

Research and working experience

- 10.2020 – current **Research scientist**, Skolkovo Institute of Science and Technology, Moscow 121205, Russian Federation *Computational study of materials for energy storage*
- 01.2018 – 12.2020 **Co-investigator**, RFBR, Grant No. 18-02-00585 A, PI Dr. Lipnitskii A.G. at BSU, Russia *Short-range order and diffusion mechanisms in concentrated solid solutions of refractory bcc metals*
- 01.2019 – 12.2019 **Engineer Research Scientist**, Laboratory of Theoretical investigations and Computer simulation, Belgorod State University, Belgorod, Russia
- Ministry of Education and Science of the Russian Federation, Contract No.3.3144.2017/PP, «Investigation of the laws and mechanisms of the formation of interfaces and structure of composite coatings on the surface of titanium alloys under the combined action of ultrashort laser pulses and arc microplasma».
- 11.2017 – 04.2018 **Engineer Research Scientist**, Institute of Strength Physics and Materials Science, Siberian Branch Russian Academy of Sciences, Tomsk, Russia
- Russian Foundation for Basic Research, Grant No. 17-308-50026 mol_nr, «A study of the primary radiation damage and the atomic mechanisms of the swelling in the V-4Ti alloy».
- 01.2014 – 12.2016 **Laboratory Assistant**, Laboratory of Theoretical investigations and Computer simulation, Belgorod State University, Belgorod, Russia
- Ministry of Education and Science of the Russian Federation, Contract No. 3.1282.2014/K, «Development of a universal model of interatomic interactions in systems with metallic and covalent bond types for the computer design of new materials with predetermined properties based on molecular dynamics and approbation of the model using the example of V-Fe-Ti system».

Scientific Interests

- Computational materials science
- High-throughput computations
- Cathode materials for Li/Na-ion battery
- Radiation-resistant alloys

Current research grants

- 01.2022 – current **co-investigator**, Russian science foundation, Grant No. 20-43-01012 FWO PI: A.M. Abakumov
Towards advanced high capacity layered electrode materials for lithium-ion batteries through understanding redox processes at the atomic level
- 10.2020 – current **co-investigator**, The Skoltech – MIT Joint Next Generation Program (NGP). Skoltech PI: Artem M. Abakumov, Center for Energy Science and Technology. MIT PI: Jennifer L.M. Rupp, Department of Materials Science and Engineering
Atomic-level Understanding of Interface Structure Evolution and Engineering Guidelines for Next Li-ion Solid State Batteries

Accomplished research grants

- 06.2019 – 06.2021 **co-investigator**, RSF Grant No. 19-73-00321 (1.5 mln.RUB/year), PI Dr. Aksyonov D.A. at Skoltech,
Search for new materials of gas electrodes for lithium and sodium-oxygen batteries: predictive computer simulation and experimental verification
- 04.2018 – 03.2020 **co-investigator**, RFBR Grant No. 18-33-00821 (0.5 mln.RUB/year), PI Dr. Aksyonov D.A. at Skoltech,
Computer modelling and experimental study of surface segregation of alloying elements for sodium-containing oxides and polyanionic compounds of transition metals
- 01.2018 – 12.2020 **co-investigator**, RFBR, Grant No. 18-02-00585 A (0.7 mln.RUB/year), PI Dr. Lipnitskii A.G. at BSU, Russia *Short-range order and diffusion mechanisms in concentrated solid solutions of refractory bcc metals*
- 11.2017 – 04.2018 **co-investigator**, RFBR, Grant No. 17-308-50026 mol_nr (0.6 mln.RUB), PI Dr. Zolnikov K.P. at ISPMS SBRAS Tomsk, Russia *A study of the primary radiation damage and the atomic mechanisms of the swelling in the V-4Ti alloy*
- 01.2017 – 12.2019 **co-investigator**, Ministry of Education and Science of the Russian Federation, Contract No. 3.3144.2017 at BSU, Russia *Investigation of the laws and mechanisms of the formation of interfaces and structure of composite coatings on the surface of titanium alloys under the combined action of ultrashort laser pulses and arc microplasma*
- 01.2014 – 12.2016 **co-investigator**, Ministry of Education and Science of the Russian Federation, Contract No. 3.1282.2014/K at BSU, Russia *Development of a universal model of interatomic interactions in systems with metallic and covalent bond types for the computer design of new materials with predetermined properties based on molecular dynamics and approbation of the model using the example of V-Fe-Ti system*

Education

- 10.2015 – 10.2019 **Candidate of Sciences in Physics and Mathematics (PhD)**, Laboratory of Theoretical investigations and Computer simulation, Belgorod State University, Belgorod, Russia
Specialty: Condensed Matter Physics
Effect of alloying on the radiation swelling of vanadium alloys
- 09.2010 – 06.2015 **Specialist in the field of nanomaterials**, Diploma with distinction (**GPA 5.00**), Belgorod State University, Belgorod, Russia
Department of Physics and Engineering
Description of the interaction between atoms in Ti-V binary system

Teaching experience

- 10.2022 - current **Organizer Assistant**, Coordination and organization of educational seminar at Skoltech
Computational Materials Science Seminar
- 2019 **Webinar lecturer**, for students
Computer modeling in materials science

Developed educational material

[DFT Crash Course](#) for School-Conference of Young Scientists at Skoltech

Online-course for students: [Atomistic modelling in materials science](#)

Online-course for students: [Nanocoatings and layered metallic nanostructures](#)

Organizing experience

- 11.2022 **Tutor**, Design and implementation of Computational Track during [VII International Conference of Young Scientists](#) at Skoltech
- 11.2021 **Tutor**, Design and implementation of Computational Track during [VI International Conference of Young Scientists](#) at Skoltech

Patents

Patent No. RU160505 U1

Computer skills

Scientific packages VASP, ABINIT, SIMAN, LAMMPS, OVITO, Jmol, Vesta
Programming Python, Fortran, Bash
General Linux OS, L^AT_EX, Office package

Scholarships

- 9.2018 – 9.2019 Scholarship of the Russian Federation Government for young scientists
- 9.2018 – 9.2019 Scholarship of the Belgorod governor for young scientists
- 9.2017 – 9.2018 Scholarship of the Belgorod governor for young scientists
- 9.2016 – 9.2017 Scholarship of the Belgorod governor for young scientists
- 9.2014 – 9.2015 Scholarship of the Russian Federation President for young scientists
- 9.2012 – 9.2013 Scholarship of the Russian Federation President for young scientists
- 9.2011 – 9.2012 Scholarship of the Russian Federation Government for young scientists

Honours and Awards

- 2018 The second degree winner of All-Russian Olympiad "Nanotechnology - a breakthrough into the future"
- 2015 The winner of the "3K Olympiad" in the area of Metallurgy
- 2015 The second degree winner of innovative projects within the framework of the international exhibition-congress "High technologies. Innovation. Investments "for the project" Portable aromatherapy device with microcontroller"
- 2015 The winner of «Student-Researcher» contest, Belgorod State University

Publications

Author or co-author of 23 published papers and 107 citations (Scopus database). H-index = 6 (7 in Google Scholar).

List of planned publications in 2022-23

Aksyonov D.A., **Boev A.O.**, Fedotov S.S., Abakumov A.M.. Computational Insights into Ionic Conductivity of Intercalation Materials for Metal-Ion Batteries - A Review. (under Review in Solid State Ionics)

Savina A.A., **Boev A.O.**, Orlova E.D., Morozov A.V., Abakumov A.M.. Ni is an element of the "green" energy of the future. (preparing for submission)

Boev A.O., Aksyonov D.A. et. al. Computational study of surface segregation in layered (Li,Na)CoO₂ oxides. (preparing for submission)

Boev A.O., Aksyonov D.A. et. al. Slow Ligand-to-Metal charge transfer in Li-excess cathode materials. (preparing for submission)

- 2022 A. Morozov, H. Paik, **A. Boev**, D. Aksyonov, S. Lipovskikh, K. Stevenson, A. Abakumov. Thermodynamics as a Driving Factor of LiCoO₂ Grain Growth on Nanocrystalline Ta-LLZO Thin Films for All-Solid-State Batteries. *ACS Applied Materials & Interfaces*, 14(35), 39907-39916 DOI:10.1021/acsami.2c07176 (IF (JCR) - 10.383 (Q1))
- A V. Morozov, I A. Moiseev, A A. Savina, **A O. Boev**, D A. Aksyonov, V A. Nikitina, E V. Antipov, A M. Abakumov. Retardation of structure densification by Ru doping in Li-rich layered oxide positive electrodes for Li-ion batteries. *Chemistry of Materials*, 34(15), 6779-6791. DOI:10.1021/acs.chemmater.2c00921 (IF (JCR) - 10.508 (Q1))
- A A. Savina, V V. Saiutina, A V. Morozov, **A O. Boev**, D A. Aksyonov, C. Dejoie, M. Batuk, S. Bals, J. Hadermann, A M. Abakumov. Chemistry, Local Molybdenum Clustering, and Electrochemistry in the Li_{2+x} Mo_{1-x} O₃ Solid Solutions. *Inorganic Chemistry*, 61(14), 5637-5652. DOI:10.1021/acs.inorgchem.2c00420 (IF (JCR) - 5.436 (Q1))
- M.R. Gazizov, **A.O. Boev**, C.D. Marioara, R. Holmestad, M.Yu. Gazizova, R.O. Kaibyshev. Edge interfaces of the Ω plates in a peak-aged Al-Cu-Mg-Ag alloy. *Materials Characterization*, 111747. DOI:10.1016/j.matchar.2022.111747 (IF (JCR) - 4.342 (Q1))
- I.V. Nelasov, A.I. Kartamyshev, **A.O. Boev**, Yu.R. Kolobov. High-speed mass transfer in the W-Cu pseudo-alloy. *Solid State Communications*, 347, 114708. DOI:10.1016/j.ssc.2022.114708 (IF (JCR) - 1.934 (Q2))
- 2021 Gazizov, M. R., **Boev, A. O.**, Marioara, C. D., Holmestad, R., Aksyonov, D. A., Gazizova, M. Y., & Kaibyshev, R. O. (2021). Precipitate/matrix incompatibilities related to the {111} Al Ω plates in an Al-Cu-Mg-Ag alloy. *Materials Characterization*, 111586. <https://pubs.acs.org/doi/full/10.1021/acsaem.1c00872> DOI:10.1016/j.matchar.2021.111586 (IF (JCR) - 4.342 (Q1))
- Abakumov A. M., Li C., **Boev A.O.**, Aksyonov D. A., Savina A. A., Abakumova T. A., Van Tendeloo G, Bals S. (2021). Grain Boundaries as a Diffusion-Limiting Factor in Lithium-Rich NMC Cathodes for High-Energy Lithium-Ion Batteries. *ACS Applied Energy Materials*, 4(7), 6777-6786. <https://pubs.acs.org/doi/full/10.1021/acsaem.1c00872> DOI:10.1021/acsaem.1c00872 (IF (JCR) - 6.024 (Q1))
- Nelasov, I. V., Kartamyshev, A. I., **Boev, A. O.**, Lipnitskii, A. G., Kolobov, Y. R., & Nguyen, T. K. (2021). Molecular dynamics simulation of the behavior of titanium under high-speed deformation. *Modelling and Simulation in Materials Science and Engineering*, 29(6), 065007. <https://iopscience.iop.org/article/10.1088/1361-651X/ac0c22/pdf> DOI:10.1088/1361-651X/ac0c22 (IF (JCR) - 2.248 (Q2))
- Boev, A. O.**, Fedotov, S. S., Stevenson, K. J., & Aksyonov, D. A. (2021). High-throughput computational screening of cathode materials for Li-O₂ battery. *Computational Materials Science*, 197, 110592. <https://www.sciencedirect.com/science/article/pii/S0927025621003190> DOI:10.1016/j.commatsci.2021.110592 (IF (JCR) - 2.863 (Q1))
- Boev, A. O.**, Nelasov, I. V., Lipnitskii, A. G., Kartamyshev, A. I., & Aksyonov, D. A. (2021). Self-point defect trapping responsible for radiation swelling reduction in V-Ti alloys. *Solid State Communications*, 329, 114252. <https://www.sciencedirect.com/science/article/pii/S0038109821000648> DOI:10.1016/j.ssc.2021.114252 (IF (JCR) - 1.804 (Q2))
- Vershinina, T. N., Bobrikov, I. A., Sumnikov, S. V., **Boev, A. O.**, Balagurov, A. M., Mohamed, A. K., & Golovin, I. S. (2021). Crystal structure and phase composition evolution during heat treatment of Fe-45Ga alloy. *Intermetallics*, 131, 107110. <https://www.sciencedirect.com/science/article/pii/S0966979521000273> DOI: 10.1016/j.intermet.2021.107110 (IF (JCR) - 3.398 (Q1))

- Gazizov M. R., **Boev A.O.**, Marioara C. D., Andersen S. J., Holmestad R., Kaibyshev R. O., Aksyonov D.A., Krasnikov V. S. The unique hybrid precipitate in a peak-aged Al-Cu-Mg-Ag alloy //Scripta Materialia. – 2021. – T. 194. – C. 113669. <https://www.sciencedirect.com/science/article/pii/S1359646220307910> DOI: 10.1016/j.scriptamat.2020.113669 (IF (JCR) - 5.079 (Q1))
- Morozov, A. V., Savina, A. A., **Boev, A. O.**, Antipov, E. V., & Abakumov, A. M. (2021). Li-based layered nickel–tin oxide obtained through electrochemically-driven cation exchange. RSC Advances, 11(46), 28593-28601. <https://pubs.rsc.org/en/content/articlehtml/2021/ra/d1ra05246b> DOI:10.1039/D1RA05246B (IF (JCR) - 3.361 (Q1))
- Leineweber, A., Becker, H., **Boev, A.**, Bobrikov, I. A., Balagurov, A. M., & Golovin, I. S. (2021). Fe₁₃Ga₉ intermetallic in bcc-base Fe–Ga alloy. Intermetallics, 131, 107059. <https://www.sciencedirect.com/science/article/pii/S0966979520309638> DOI: 10.1016/j.intermet.2020.107059 (IF (JCR) - 3.398 (Q1))
- Boev A.O.**, Fedotov, S. S., Abakumov, A. M., Stevenson, K. J., Henkelman, G., & Aksyonov, D. A. (2021). The role of antisite defect pairs in surface reconstruction of layered AMO₂ oxides: A DFT+U study. Applied Surface Science, 537, 147750. <https://www.sciencedirect.com/science/article/pii/S0169433220325071> DOI:10.1016/j.apsusc.2020.147750 (IF (JCR) - 6.182 (Q1))
- 2020 **Boev A.O.**, Poletaev D.O., Kartamyshev A.I., Boeva M.V., Vershinina T.N. Influence of Mo₁₀Ni₃C₃B phase on hardness and fracture toughness of Mo-Ni-C-B cermet: an experimental and theoretical study / Letters on materials, 2020, 10(4) 387-391 <https://lettersonmaterials.com/en/Readers/Article.aspx?aid=32862> DOI: 10.22226/2410-3535-2020-4-387-391 IF (SJR) - 0.259 (Q3)
- Kartamyshev A. I., Lipnitskii A. G., **Boev A.O.**, Nelasov I., Maksimenko V. N., Aksyonov D. A., Nguyen T. K. Angular dependent interatomic potential for Ti–V system for molecular dynamics simulations //Model. and Simul. in Mat. Sci. and Eng. – 2020. – T. 28. – 5. <https://iopscience.iop.org/article/10.1088/0965-0393/ab8863/meta> DOI: 10.1088/1361-651X/ab8863 (IF - 1.874 (Q2))
- Vershinina T. N., **Boev A. O.**, Ivanov M. B. Crystal structure of a new Mo₁₀Ni₃C₃B phase //Vacuum. – 2020. – C. 109034. <https://www.sciencedirect.com/science/article/pii/S0042207X19322882>; DOI: 10.1016/j.vacuum.2019.109034 (IF (JCR) - 2.515 (Q1/Q2))
- 2019 **Boev A.O.**, Zolnikov K.P., Nelasov I.V., Lipnitskii A.G. Molecular dynamics simulation of primary radiation damage in vanadium and alloy V-4Ti //Journal of Physics: Conference Series. – IOP Publishing, 2019. – T. 1147. – No. 1. – C. 012087.
- 2018 **Boev A.O.**, Zolnikov K.P., Nelasov I.V., Lipnitskii A.G. Molecular dynamics simulation of primary radiation damage in vanadium and alloy V-4Ti /Journal of Physics: Conference Series. – AIP Publishing, 2018. – T. 8. – No.3. – C. 263-267.
- 2017 **Boev A.O.**, Aksyonov D.A., Kartamyshev A.I., Maksimenko V.N., Nelasov I.V., Lipnitskii A.G. Interaction of Ti and Cr atoms with point defects in bcc vanadium: A DFT study / Journal of Nuclear Materials, 2017, Vol. 492, P. 14-21 <http://www.sciencedirect.com/science/article/pii/S0022311516312417> ; DOI - 10.1016/j.jnucmat.2017.04.046 ; (IF - JCR - 2.536 (Q1))
- Boev, A.O.**, Nelasov, I.V., Maksimenko, V.N., Lipnitskii, A.G., Saveliev, V.N., Kartamyshev, A.I. Molecular Dynamics Simulations of the Excess Vacancy Evolution in V and V-4Ti / Defect and Diffusion Forum. – Trans Tech Publications, 2017. – T. 375. – C. 153-166.
- Boev, A. O.**, Lipnitskii, A. G., Nelasov, I. V., Saveliev, V. N., Kartamyshev, A. I., Maksimenko, V. N., Zolnikov, K. P. Molecular dynamic simulations of the interaction of interstitial atoms with vacancy complexes in V and V-4Ti /AIP Conference Proceedings, 2017. – T. 1909. – 1.

- 2019 Aksyonov D. A., **Boev A. O.**, Fedotov S. S., Stevenson K. J. Surface Energy and Reconstruction of Li and Na Based Transition Metal Oxides: A Computational Study //Meeting Abstracts. – The Electrochemical Society, 2019. – No. 4. – C. 207-207.
- 2017 Maksimenko V. N., **Boev A. O.**, Lipnitskii A. G., Saveliev V. N., Kartamyshev A.I. Chromium interatomic potentials for modeling //Nuclear physics and engineering, 2017. – T. 8 - No. 1. – C. 69-75.[in Russian]
- Boev A. O.**, Nelasov I.V., Maksimenko V. N., Lipnitskii, A. G., Saveliev, V. N., Kartamyshev A.I. Molecular dynamics simulation of the formation of excess vacancies complexes in V and V-4Ti //Nuclear physics and engineering, 2017. – T. 8 - No. 1. – C. 145-149.[in Russian]
- 2016 Kartamyshev A.I., **Boev A.O.**, et al. Many-body interatomic potentials in Ti-V system with angular dependence for molecular dynamics simulations/ BSU Scient. bullet. : Math. and Phys. 121 67–78 (2016). [In Russian]
- Nelasov I.V., **Boev A.O.**, Lipnitskii A.G. Study of Cu/Nb interface diffusion by molecular dynamics simulation / XV International conference on intergranular and interphase boundaries in materials (iib-2016) Book of abstracts. 2016. C. 96.
- 2014 **Boev A.O.**, Lipnitskii A.G. Equilibrium and stability of triple junction in nanolayer Cu/Nb / BSU Scient. bullet. : Experimental & Applied Physics. 7 (178) 2014. [In Russian]

List of Talks

- 2022 Oral talk "The role of twin boundaries in lithium-enriched layered cathode materials", IV Baikal materials forum in Ulan-Ude, Russia, 01.07.2022-07.07.2022
- 2021 Oral talk "The role of antisite defect pairs in surface reconstruction of layered AMO₂ oxides: A DFT+U study", X National Crystal Chemical Conference in Terskol, Russia, 05.08.2021-10.08.2021
- 2019 Poster "Surface reconstruction of Li and Na based transition metal oxides: A DFT study", Inaugural Symposium for Computational Materials Program of Excellence (cmp.skoltech.ru) in Moscow, Russia, 04.09.2019-08.09.2019, poster session
- 2018 Poster "Surface reconstruction of Li and Na based transition metal oxides: A DFT study", XXXIII International Conference on Equations of State for Matter March 1–6, 2018, Elbrus, Kabardino-Balkaria, Russia
- 2017 Oral talk "Diffusion characteristics of self-point defects in V-4Ti alloy", XIV Kurchatov interdisciplinary youth scientific school, 14.11.2017-17.11.2017, Moscow, Russia, oral session
- 2016 Oral talk "Molecular dynamics study of excess vacancy complexes evolution in V and V-4Ti", XV Kurchatov interdisciplinary youth scientific school, 8.11.2016-11.11.2016, Moscow, Russia, oral session
- 2016 Oral talk "Binding energies of Ti and Cr atoms with vacancies and interstitial atoms in bcc vanadium", XXIII International Conference of Students, Postgraduates and Young Scientists in Basic Sciences "Lomonosov-2016", 11.04.2016-15.04.2016, Moscow, Russia, oral session
- 2013 Poster "Equilibrium and stability of triple junctions in Cu-Nb nanolaminate", V All-Russian youth conference on fundamental and innovative issues of modern physics, 10.11.2013-15.11.2013, Moscow, Russia, poster session