Daniil Poletaev

ORCID: 0000-0003-3057-3427; WoS ResearcherID: F-6862-2016; Scopus Author ID: 56380377900

Personal information

Date of Birth	October 24, 1990
Sex	Male
Family status	Married, three children
Citizenship	Russia
Languages	English (intermediate), Russian (native speaker)

Education

09.2012–02.2017 **Candidate of Sciences in Physics and Mathematics (PhD)**, Laboratory of Theoretical investigations and Computer simulation, Belgorod State University, Belgorod, Russia.
Speciality: Condensed Matter Physics
Thesis: *Prediction of hydrogen and silicon solubility in an α-Ti within the density functional theory*

09.2007–06.2012 **Specialist in the field of nanomaterials**, Belgorod State University, Belgorod, Russia.
Department of Physics and Engineering
Thesis: *Methods of molecular dynamics and density functional theory in the studying of the phase transitions in metallic systems on the example of Ti and Cu-Nb composite*

Working experience

2022–present **Research Scientist**, *Materials Discovery Laboratory, Skolkovo Institute of Science and Technology, Moscow, Russia*.
RSCF project No. 19-72-30043 "Computational materials design laboratory", ab initio calculations of superconducting critical temperature in the predicted materials with account of anharmonic contributions, development of finite-temperature structure prediction methods, computational search for new promising hard magnets, Supervisor - Oganov A.R.

2022–2025 **Senior Research Scientist**, *Laboratory of Theoretical investigations and Computer simulation, Belgorod State University, Belgorod, Russia*.
RSCF project No. 22-72-10026, "Theoretical prediction of radiation swelling and diffusion in promising metallic materials for nuclear power based on atomistic modeling on the example of vanadium alloys of the V-Zr-Ti-Cr-W-C system", Supervisor - Poletaev D.O.

2022–2023 **Research Scientist**, *Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russia*.
Ab initio investigations of coherent cluster ordering in magnetostrictive materials of Fe-Ga-Al system, Supervisor - Balagurov A.M.

2019–2021 **Research Scientist**, *Laboratory of Theoretical investigations and Computer simulation, Belgorod State University, Belgorod, Russia*.
– Russian Science Foundation, Grant No. 19-73-00313, "Development of an approach to constructing of phase diagrams of materials with metallic and covalent bond types within the CALPHAD on the basis of experimental data and results of atomistic modeling using the example of the Ti-Si-H system. ", Senior researcher - Poletaev D.O.

2011–2019 **Programmer**, *Belgorod virtual branch of the Russian Museum, Belgorod State Institute of Arts and Culture, Belgorod, Russia*.

2014–2016 **Junior Scientist**, *Laboratory of Theoretical investigations and Computer simulation, Belgorod State University, Belgorod, Russia*.
– Ministry of Education of Russian Federation, Grant No. 3.1282.2014/K, "Development of an universal model of interatomic interactions in systems with metallic and covalent types of bonding for the computer design of new materials with predetermined properties within the molecular dynamics, and approbation of the model using the vanadium-iron-titanium system as an example", Senior researcher - Lipnitskii A.G.

2012–2015 **Junior Scientist**, *Laboratory of Theoretical investigations and Computer simulation, Belgorod State University, Belgorod, Russia*.
– Ministry of Education of Russian Federation, Contract No. 02.G25.31.0103, "Development of the technology for the creation of porous bioactive nanostructured coatings on the surface of elements of hip and knee endoprostheses made from titanium alloys that have controlled pore space, specified relief parameters and biochemical activity", Senior researcher - Kolobov Yu.R.

Research interests

, Computational search for new inorganic materials. Refinement and extension of phase diagrams of inorganic materials with metallic and covalent types of bonding by calculation of the thermodynamic properties of solid phases within the density functional theory, atomistic simulations with semiempirical and machine-learning interatomic potentials, and CALPHAD approach. Investigation of grain boundary segregation and diffusion characteristics of impurities in metals within the density functional theory. Construction of semiempirical and machine-learning nteratomic potentials. Anharmonic calculations of superconductuvity, thermal conductivity and other phonon related properties of materials. Development of automated or semi-automated pipelines for computational materials design from crystal structure prediction to practical guidelines for materials manufacturing.

Computer skills

Scientific packages	ABINIT, VASP, Wien2k, LAMMPS, Thermocalc, Pymatgen, Siman, SSCHA, MLIP
Programming	Python, Fortran, C++, Bash, HTML
General	Experienced user of Windows, Linux OS and LaTeX
Github	https://github.com/Kurufinve

List of the most important publications

[1] A.G. Lipnitskii, V.N. Maksimenko, A.V. Vyazmin, A.I. Kartamyshev, and **D.O. Poletaev**. A new method of calculation of the thermodynamic properties of point defects in concentrated solid solutions: An application to VNbMoTaW alloy. *Computational Materials Science*, 256(April):113945, jun 2025.

[2] V.N. Maksimenko, A.G. Lipnitskii, V.N. Saveliev, A.I. Kartamyshev, A.V. Vyazmin, and **D.O. Poletaev**. N-body interatomic potential for molecular dynamics simulations of V-Cr-Nb-Mo-Ta-W system. *Computational Materials Science*, 247(November 2024):113533, jan 2025.

[3] A.I. Kartamyshev, A.G. Lipnitskii, I.G. Chepelev, A.V. Vyazmin, and **D.O. Poletaev**. The N-body interatomic potential for carbon: Influence of the precision of three-body interactions' contribution on the accuracy of molecular dynamics simulations. *Computational Materials Science*, 242(May):113100, jun 2024.

[4] A.V. Vyazmin, A.G. Lipnitskii, A.I. Kartamyshev, V.N. Maksimenko, and **D.O. Poletaev**. N-body potential for simulation of α and β phases of zirconium. *Computational Materials Science*, 235:112806, feb 2024.

[5] A. V. Vyazmin, A. G. Lipnitskii, V. N. Maksimenko, **D.O.** textbfPoletaev, and A. I. Kartamyshev. Molecular dynamics simulation of diffusion along general high-angle grain boundaries in copper and vanadium. *Letters on Materials*, 13(4s):450–455, 2023.

[6] A.I. Kartamyshev, **D.O. Poletaev**, A.O. Boev, and D.A. Aksyonov. Weak segregation and accelerated diffusion of Li at twin boundaries in Cu from DFT: Implications for current collectors in Li-ion batteries. *Computational Materials Science*, 230(September):112517, oct 2023.

[7] A.I. Kartamyshev, A.G. Lipnitskii, V.N. Maksimenko, A.V. Vyazmin, I.V. Nelasov, and **D.O. Poletaev**. N-body potential for simulating lattice defects and diffusion in copper. *Computational Materials Science*, 228(May):112284, sep 2023.

[8] **D.O. Poletaev**, A.G. Lipnitskii, V.N. Maksimenko, Yu.R. Kolobov, A.G. Beresnev, and M.S. Gusakov. The N-body interatomic potentials for molecular dynamics simulations of diffusion in C15 Cr2Ta Laves phase. *Computational Materials Science*, 216(June 2022):111841, jan 2023.

[9] M. Ait Boukideur, N. Selhaoui, F.Z. Chrifi Alaoui, **D.O. Poletaev**, H. Bouchta, K. Achgar, and A. Aharoune. Thermodynamic assessment of the Ga–Lu system bythe combination of ab-initio calculations and the CALPHAD approach. *Calphad*, 79(March):102464, dec 2022.

[10] V. N. Maksimenko, A. G. Lipnitskii, A. I. Kartamyshev, **D. O. Poletaev**, and Yu R. Kolobov. The N-body interatomic potential for molecular dynamics simulations of diffusion in tungsten. *Computational Materials Science*, 202(October 2021):110962, 2022.

[11] **D.O. Poletaev**, D.A. Aksyonov, and A.G. Lipnitskii. Evolutionary search for new compounds in the Ti–Si system. *Calphad*, 71:102201, dec 2020.

[12] Anton Boev, **Daniel Poletaev**, Andrey Kartamyshev, Mariya Boeva, and Tatiana Vershinina. Influence of the Mo10Ni3C3B phase on the hardness and fracture toughness of Mo-Ni-C-B cermet: experimental and theoretical study. *Letters on Materials*, 10(4):387–391, 2020.

[13] A.I. Kartamyshev, **D.O. Poletaev**, and A.G. Lipnitskii. The influence of lattice vibrations and electronic free energy on phase stability of titanium silicides and Si solubility in hcp titanium: A DFT study. *Calphad*, 65(February):194–203, jun 2019.

[14] A.I. Kartamyshev, A.G. Lipnitskii, V.N. Saveliev, V.N. Maksimenko, I.V. Nelasov, and **D.O. Poletaev**. Development of an interatomic potential for titanium with high predictive accuracy of thermal properties up to melting point. *Computational Materials Science*, 160:30–41, apr 2019.

[15] **D.O. Poletaev**, D.A. Aksyonov, Dat Duy Vo, and A.G. Lipnitskii. Hydrogen solubility in hcp titanium with the account of vacancy complexes and hydrides: A DFT study. *Computational Materials Science*, 114:199–208, 2016.

[16] **D.O. Poletaev**, A.G. Lipnitskii, A.I. Kartamyshev, D.A. Aksyonov, E.S. Tkachev, S.S. Manokhin, M.B. Ivanov, and Yu. R. Kolobov. Ab initio-based prediction and TEM study of silicide precipitation in titanium. *Computational Materials Science*, 95:456–463, 2014.

Conferences

1. Inaugural Symposium for “Computational Materials Program of Excellence”, 04 – 06 September 2019, Skoltech, Russia (https://cmp.skoltech.ru/) - poster presentation
2. International Conference on Computer Coupling of Phase Diagrams and Thermochemistry "CALPHAD GLOBAL", June 2021, World Wide Web (https://calphad.org/calphad-global-home) - online poster presentation
3. SSCHA School 2023, June 2023, Donostia/San Sebastián, Spain - oral presentation
4. First All-Russian Conference on Computational Materials Science, October 30 - November 2, 2023, Skoltech, Russia - poster presentation
5. 2nd Sino-Russian Symposium on Chemistry and Materials, May 29 - June 1, 2024, Skoltech, Russia - poster presentation