

CURRICULUM VITAE (December 24, 2018)
ALEXANDER G. KVASHNIN

Personal data

Born on 05.08.1989 in Krasnoyarsk, Russia
Married, two children
Languages: English (fluent), Russian (native)

ORCID: <http://orcid.org/0000-0002-0718-6691>

Scopus Author ID: 6603118309

[Google Scholar page](#)

Education

2016 Ph.D. in condensed matter physics (Moscow Institute of Physics and Technology)
2012 M.Sc. in Applied Mathematics and Physics (Moscow Institute of Physics and Technology)
2010 B.Sc. in physics (Siberian Federal University)

Employment

2017-present Senior Research Scientist, Skolkovo Institute of Science and Technology, Moscow
2016-2017 Research Scientist, Skolkovo Institute of Science and Technology, Moscow
2015-2016 Junior Research Scientist, Skolkovo Institute of Science and Technology, Moscow
2013-2015 Junior Research Scientist, Technological Institute for Superhard and Novel Carbon Materials (TISNCM), Troitsk
2012-2015 Administrator of HPC cluster, Technological Institute for Superhard and Novel Carbon Materials (TISNCM), Troitsk
2010-2012 Research Intern, Technological Institute for Superhard and Novel Carbon Materials (TISNCM), Troitsk

Ph.D. Advisor: Pavel B. Sorokin, (TISNCM)

Postdoctoral Advisor: Artem R. Oganov, Skoltech

Student Supervisions: Dmitrii V. Semenok (2018 –)

Visiting Appointments: Visiting International Scholar in Rice University, 2011; Visiting International Scientist in Rice University, 2013; Visiting PhD students, University of Namur, 2015; Visiting Professor, Northwestern Polytechnical University, Xi'an, 2018.

Citations Summary: h-index: 9 (WoS), 9 (Scopus), 11 (Google Scholar); Citation: 1402 (WoS), 1443 (Scopus), 1856 (Google Scholar)

Research Interests/Expertise

Computational search for novel materials of various dimensionalities with optimal and unique physical and chemical properties. Characterization of physical and chemical properties of different materials in terms of crystal structure, electronic structure, and physical properties using modern quantum chemical and molecular dynamics methods. 2D materials, surfaces, clusters, superhard and ultrahard materials, electrochemical storage, superconductivity.

Honors and Awards

- 2013-2015 Scholarship of President of Russia for young scientists and PhD students
2010-2012 Scholarship of the “Dynasty” foundation
2010 Scholarship for achievements in the field of Mathematical and Physical Sciences
2009 President Scholarship for students
2009 Diploma laureate head of the Krasnoyarsk city for young talent for excellence in scientific and educational activities

Grants and Projects

- 2019-2020 Russian Foundation of Basic Research project № 19-03-00100, “Study of superconductivity with electron-phonon coupling mechanism in hydrides, borides and carbides of transition metals stabilized by pressure” (**leader**)
2018-2019 UMNIK program, Light elements: superconducting ternary systems with light elements (**leader**)
2017-2019 Industry project with OOO "Gazpromneft' NTC", “Design new superhard materials for the cutters of the drill bit, and their subsequent synthesis and testing”
2017-2020 Russian Science Foundation project № 17-73-20038, “Computational design for new materials with optimal hardness and fracture toughness” (**leader**)
2016-2018 Russian Science Foundation project № 16-13-10459. New methods for search for materials with optimal properties (participant)
2014-2016 Russian Science Foundation project № 14-12-01217. Simulations of structure and properties of new multilayered nanomaterials based on TMDs and BN-graphene layered structures (participant)
2012-2015 Research project of Federal Target program № 14.B37.21.1645. Investigation of fabrication ways and properties of single-crystal diamond film with nanometer thickness (participant)
2012-2015 Russian Foundation of Basic Research program № 12-02-31261. Investigation of features of electronic, elastic and mechanical properties of materials based on diamond clusters with nanometer size (participant)

Assigner Reviewer

The Journal of Chemical Physics; Computational Materials Science; 2D Materials; Journal of Applied Physics; The Journal of Physical Chemistry Letters, Carbon.

Synergistic Activities

Education and Training. Workshops organized: “Trends in nanomechanics and nanoengineering” Co-organizer with Sorokin.

BOOKS

1. A.R. Oganov, G. Saleh, **A.G. Kvashnin** (Editors). Computational Materials Discovery. Royal Society of Chemistry. ISBN: 978-1-78262-961-0. (2018)

PAPERS IN REFEREED JOURNALS

- 37 I.A. Kruglov, D.V. Semenov, R. Szczeniak, M.M. Davari Eshafani, **A.G. Kvashnin** and A.R. Oganov, Superconductivity in LaH₁₀: a new twist of the story, *ArXiv1810.01113* (2018)
- 36 D.V. Semenov, I.A. Kruglov, **A.G. Kvashnin** and A.R. Oganov, On Distribution of Superconductivity in Metal Hydrides, *ArXiv1806.00865* (2018)
- 35 A. Kartsev, O. Feya, N. Bondarenko, **A.G. Kvashnin** and A.R. Oganov, Stability and magnetism of FeN high-pressure phases, *ArXiv1806.00874* (2018)
- 34 **A.G. Kvashnin**, D. V. Semenov, I. A. Kruglov and A. R. Oganov, High-Temperature Superconductivity in Th-H System at Pressure Conditions, *ACS Appl. Mater. Interfaces*, 10, 50, 43809-43816 (2018) (DOI: [10.1021/acsami.8b17100](https://doi.org/10.1021/acsami.8b17100))
- 33 A.I. Kruglov, **A.G. Kvashnin**, A.F. Goncharov, A.R. Oganov, S.S. Lobanov, N. Holtgrewe, S. Jiang, V.B. Prakapenka, E. Greenberg and A.V. Yanilkin, Uranium polyhydrides at moderate pressures: prediction, synthesis, and expected superconductivity, *Sci. Adv.* 4, 10, eaat9776 (2018) (DOI: [10.1126/sciadv.aat9776](https://doi.org/10.1126/sciadv.aat9776)).
- 32 **A.G. Kvashnin**, H.A. Zakaryan, C. Zhao, Y. Duan, Yu.A. Kvashnina, C. Xie, H. Dong, A.R. Oganov, New Tungsten Borides, Their Stability and Outstanding Mechanical Properties, *J. Phys. Chem. Lett.* 9, 3470-3477 (2018) (DOI: [10.1021/acs.jpcclett.8b01262](https://doi.org/10.1021/acs.jpcclett.8b01262))
- 31 D.V. Semenov, **A.G. Kvashnin**, I.A. Kruglov, A.R. Oganov, Actinium Hydrides AcH₁₀, AcH₁₂, AcH₁₆ as High-Temperature Conventional Superconductors, *J. Phys. Chem. Lett.* 8, 1920-1926 (2018) (DOI: [10.1021/acs.jpcclett.8b00615](https://doi.org/10.1021/acs.jpcclett.8b00615))
- 30 **A.G. Kvashnin**, I.A. Kruglov, D.V. Semenov, A.R. Oganov, Iron Superhydrides FeH₅ and FeH₆: Stability, Electronic Properties, and Superconductivity, *J. Phys. Chem. C*, 122 (8), pp 4731-4736 (2018) (DOI: [10.1021/acs.jpcc.8b01270](https://doi.org/10.1021/acs.jpcc.8b01270))
- 29 **A.G. Kvashnin**, P.B. Sorokin, L.A. Chernozatonskii, Layered heterostructures based on graphene, hexagonal zinc oxide and molybdenum disulfide: Modeling of geometry and electronic properties, *Comp. Mat. Sci.*, 142, 32-37 (2018) (DOI: [10.1016/j.commatsci.2017.09.040](https://doi.org/10.1016/j.commatsci.2017.09.040))
- 28 **A.G. Kvashnin**, P.V. Avramov, D.G. Kvashnin, L.A. Chernozatonskii, P.B. Sorokin, Features of Electronic, Mechanical, and Electromechanical Properties of Fluorinated Diamond Films of Nanometer Thickness, *J. Phys. Chem. C.*, 121, 28484-28489 (2017) (DOI: [10.1021/acs.jpcc.7b07946](https://doi.org/10.1021/acs.jpcc.7b07946))
- 27 H.A. Zakaryan, **A.G. Kvashnin**, A.R. Oganov, Stable reconstruction of the (110) surface and its role in pseudocapacitance of rutile-like RuO₂, *Sci. Rep.*, 7, 10357 (2017) (DOI: [10.1038/s41598-017-10331-z](https://doi.org/10.1038/s41598-017-10331-z))
- 26 Yu.A. Kvashnina, D.G. Kvashnin, **A.G. Kvashnin**, P.B. Sorokin, New allotropic forms of carbon based on C₆₀ and C₂₀ fullerenes with specific mechanical characteristics, *JETP Lett.*, 105, 419-425 (2017) (DOI: [10.1134/S0021364017070104](https://doi.org/10.1134/S0021364017070104))
- 25 **A.G. Kvashnin**, A.R. Oganov, A.I. Samtsevich, Z. Allahyari, Computational Search for Novel Hard Chromium-Based Materials, *J. Phys. Chem. Lett.*, 8, 755-764 (2017) (DOI: [10.1021/acs.jpcclett.6b02821](https://doi.org/10.1021/acs.jpcclett.6b02821))
- 24 D.G. Kvashnin, O.P. Kvashnina, P.V. Avramov, P.B. Sorokin, **A.G. Kvashnin**, Novel hybrid C/BN two-dimensional heterostructures, *Nanotechnology*, 28, 085205 (2017) (DOI: [10.1088/1361-6528/aa55e9](https://doi.org/10.1088/1361-6528/aa55e9))
- 23 Yu.A. Kvashnina, **A.G. Kvashnin**, L.A. Chernozatonskii, P.B. Sorokin, Fullerite-based nanocomposites with ultrahigh stiffness. Theoretical investigation, *Carbon*, 115, 546-549 (2017) (DOI: [10.1016/j.carbon.2017.01.028](https://doi.org/10.1016/j.carbon.2017.01.028))

- 22 **A.G. Kvashnin**, P.V. Avramov, S. Sakai, Yu.S. Nechaev, P.B. Sorokin, Estimation of graphene surface stability against the adsorption of environmental and technological chemical agents, *Phys. Stat. Sol. B*, 254, 6, 1600702 (2017) (DOI: [10.1002/pssb.201600702](https://doi.org/10.1002/pssb.201600702))
- 21 L.Yu. Antipina, **A.G. Kvashnin**, P.B. Sorokin, L.A. Chernozatonskii, The possible formation of magnetic FeS₂ phase in two-dimensional MoS₂ matrix, *Phys. Chem. Chem. Phys.*, 18, 26956-26959 (2016) (DOI: [10.1039/C6CP05065D](https://doi.org/10.1039/C6CP05065D))
- 20 L.A. Chernozatonskii, **A.G. Kvashnin**, P.B. Sorokin, Heterostructures based on graphene and MoS₂ layers decorated by C₆₀ fullerenes, *Nanotechnology*, 27, 365201-365206 (2016) (DOI: [10.1088/0957-4484/27/36/365201](https://doi.org/10.1088/0957-4484/27/36/365201))
- 19 **A.G. Kvashnin**, E.Y. Pashkin, B.I. Yakobson, P.B. Sorokin, Ionic Graphitization of Ultrathin Films of Ionic Compounds, *J. Phys. Chem. Lett.* 7, 2659–2663 (2016) (DOI: [10.1021/acs.jpcllett.6b01214](https://doi.org/10.1021/acs.jpcllett.6b01214))
- 18 **A.G. Kvashnin**, P.B. Sorokin, B.I. Yakobson, Flexoelectricity in Carbon Nanostructures: Nanotubes, Fullerenes, and Nanocones, *J. Phys. Chem. Lett.* 6, 2740–2744 (2015) (DOI: [10.1021/acs.jpcllett.5b01041](https://doi.org/10.1021/acs.jpcllett.5b01041)).
- 17 **A.G. Kvashnin**, O.P. Kvashnina, D.G. Kvashnin, Hydrogen adsorption study. Formation of quantum dots on graphene nanoribbons within tight-binding approach, *Nanotechnology*, 26, 175704-175708 (2015) (DOI: [10.1088/0957-4484/26/17/175704](https://doi.org/10.1088/0957-4484/26/17/175704))
- 16 Yu.A. Kvashnina, **A.G. Kvashnin**, M.Yu. Popov, B.A. Kulnitskiy, I.A. Perezhogin, E.V. Tyukalova, L.A. Chernozatonskii, P.B. Sorokin and V.D. Blank, Toward the Ultra-incompressible Carbon Materials. Computational Simulation and Experimental Observation, *J. Phys. Chem. Lett.* 6, 2147–2152 (2015) (DOI: [10.1021/acs.jpcllett.5b00748](https://doi.org/10.1021/acs.jpcllett.5b00748)).
- 15 P.B. Sorokin, **A.G. Kvashnin**, Z. Zhu, D. Tománek, Spontaneous Graphitization of Ultrathin Cubic Structures: A Computational Study, *Nano Letters*, 14, 7126-7130 (2014) (DOI: [10.1021/nl503673q](https://doi.org/10.1021/nl503673q)).
- 14 **A.G. Kvashnin**, P.B. Sorokin, D. Tománek, Graphitic phase of NaCl. Bulk properties and nanoscale stability, *J. Phys. Chem. Lett.*, 5, pp. 4014–4019 (2014) (DOI: [10.1021/jz502046f](https://doi.org/10.1021/jz502046f)).
- 13 Y. Sun, **A.G. Kvashnin**, P.B. Sorokin, B.I. Yakobson, W.E. Billups, Radiation-Induced Nucleation of Diamond from Amorphous Carbon: Effect of Hydrogen, *J. Phys. Chem. Lett.* 5, pp. 1924–1928 (2014) (DOI: [10.1021/jz5007912](https://doi.org/10.1021/jz5007912)).
- 12 **A.G. Kvashnin**, L.A. Chernozatonskii, B.I. Yakobson, P.B. Sorokin, Phase Diagram of Quasi-Two-Dimensional Carbon, From Graphene to Diamond, *Nano Lett.*, 14 (2), pp 676–681 (2014) (DOI: [10.1021/nl403938g](https://doi.org/10.1021/nl403938g)).
- 11 **A.G. Kvashnin**, P.B. Sorokin, Lonsdaleite Films with Nanometer Thickness, *J. Phys. Chem. Lett.*, 5, pp 541–548 (2014) (DOI: [10.1021/jz402528q](https://doi.org/10.1021/jz402528q)).
- 10 Yu.A. Kvashnina, **A.G. Kvashnin**, P.B. Sorokin, Investigation of new superhard carbon allotropes with promising electronic properties, *J. Appl. Phys.* 114, 183708 (2013) (DOI: [10.1063/1.4829002](https://doi.org/10.1063/1.4829002))
- 9 L.A. Chernozatonskii, D.G. Kvashnin, P.B. Sorokin, **A.G. Kvashnin**, J.W. Brüning, Strong Influence of Graphene Island Configurations on the Electronic Properties of a Mixed Graphene/Graphane Superlattice, *J. Phys. Chem. C.*, 116 (37), 20035-20039 (2012) (DOI: [10.1021/jp304596y](https://doi.org/10.1021/jp304596y))
- 8 L.A. Chernozatonskii, P.B. Sorokin, A.A. Kuzubov, B.P. Sorokin, **A.G. Kvashnin**, D.G. Kvashnin, P.V. Avramov, B.I. Yakobson, Influence of Size Effect on the Electronic and Elastic Properties of Diamond Films with Nanometer Thickness, *J. Phys. Chem. C.*, 115 (1), pp 132–136, (2011) (DOI: [10.1021/jp1080687](https://doi.org/10.1021/jp1080687)).
- 7 **A.G. Kvashnin**, P.B. Sorokin, D.G. Kvashnin, The Theoretical Study of Mechanical Properties of Graphene Membranes, Fullerenes, Nanotubes and Carbon Nanostructures, 18, 4-6, 497-500, (2010) (DOI: [10.1080/1536383X.2010.488160](https://doi.org/10.1080/1536383X.2010.488160)).

- 6 L. Song, L. Ci, H. Lu, P.B. Sorokin, C. Jin, J. Ni, **A.G. Kvashnin**, D.G. Kvashnin, J. Lou, B.I. Yakobson, P.M. Ajayan, Large Scale Growth and Characterization of Atomic Hexagonal Boron Nitride Layers, *Nano Letters*, 10 (8), 3209-3215, (2010) (DOI:[10.1021/nl1022139](https://doi.org/10.1021/nl1022139)).
- 5 P. B. Sorokin, **A. G. Kvashnin**, D. G. Kvashnin, J. A. Filicheva, P. V. Avramov, A. S. Fedorov and L. A. Chernozatonskii, Theoretical Study of Atomic Structure and Elastic Properties of Branched Silicon Nanowires, *ACS Nano*, 4, N5, 2784-2790 (2010), (DOI: [10.1021/nn9018027](https://doi.org/10.1021/nn9018027)).
- 4 P.B. Sorokin, D.G. Kvashnin, **A.G. Kvashnin**, P.V. Avramov, L.A. Chernozatonskii, Theoretical Study of Elastic Properties of SiC Nanowires of Different Shapes, *J. Nanosci. Nanotechnol.* 10, 4992-4997 (2010), (DOI: [10.1166/jnn.2010.2424](https://doi.org/10.1166/jnn.2010.2424)).
- 3 **A.G. Kvashnin**, P.B. Sorokin, D.G. Kvashnin, Theoretical Investigation of Mechanical Properties of Graphene Membranes by Means of Molecular Mechanics, *Journal of Siberian Federal University. Mathematics & Physics*, 2(4), pp. 426-431 (2009).
- 2 L.A. Chernozatonskii, P.B. Sorokin, **A.G. Kvashnin** and D.G. Kvashnin, Diamond-like C₂H nanolayer, diamane: Simulation of the structure and properties. *JETP Letters*, 90 2 pp. 134-138 (2009) (DOI:[10.1134/S0021364009140112](https://doi.org/10.1134/S0021364009140112)).
- 1 P.B Sorokin, P.V. Avramov, **A.G. Kvashnin**, D.G. Kvashnin, S.G. Ovchinnikov. Density functional study of <110> oriented thin silicon nanowires. *Phys. Rev. B* 77, 235417 (2008) (DOI: [10.1103/PhysRevB.77.235417](https://doi.org/10.1103/PhysRevB.77.235417)).