

## CURRICULUM VITAE OF PAVEL B. SOROKIN

Name: **Pavel B. Sorokin**

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Date and Place of birth: **August 19, 1982, USSR**

Nationality: **Russia**



### Education (degrees, dates, universities):

Date	Degree	University
2003	Bachelor of physic *	Krasnoyarsk State University, Krasnoyarsk, Russia
2005	Master of physic **	Krasnoyarsk State University, Krasnoyarsk, Russia
2007	Doctor of philosophy ***	Lebedev Physical Institute of RAS, Moscow, Russia
2014	Habilitation ****	Karpov Institute of Physical Chemistry, Moscow, Russia

\* Ab-initio calculations of carbon nanotubes structure and properties

\*\* New non-carbon dioxide silicon and oxide berillium structures investigation

\*\*\* New nanostructures simulation by density functional method

\*\*\*\* Theoretical investigations of physical-chemical properties of low-dimensional structures

**Citation index:** 2555, **h-index:** 19 ([Google Scholar](#))

Scopus	Researcher ID	ORCID
<a href="#">9277558700</a>	<a href="#">C-9749-2011</a>	<a href="#">0000-0001-5248-1799</a>

**Specialization:** Numerical quantum chemistry, ab-initio calculations, carbon (graphene, nanotubes, ultrahard carbon materials) & noncarbon (2D inorganic films), nanostructures, nanotechnology.

### Reviewer

Nano Letters, Advanced Materials, Applied Physics Letters, Physical Status Solidi (in top 100 referee list of 2010/2011. [http://onlinelibrary.wiley.com/journal/10.1002/%28ISSN%291521-3951/homepage/pss\\_Top100\\_Refs.html](http://onlinelibrary.wiley.com/journal/10.1002/%28ISSN%291521-3951/homepage/pss_Top100_Refs.html)), Nanoscale, Physical Chemistry Chemical Physics, Computational Materials Science

### Computing Skills

**Software packages:** Molecular modeling (HyperChem, LAMMPS, GULP), ab initio quantum-mechanical calculations (VASP, Siesta, Abinit, PWSCF), Semi-empirical calculations (GAMESS, HyperChem), Tight-binding calculations (deMon).

**Languages:** Fortran 90/95, C/C++, MatLab, HTML

**Operating Systems:** MS Windows, Linux

**Software Applications:** Scientific computing/visualization tools (Matlab, Maple, [SigmaPlot](#), [Diamond](#), [Chemcraft](#), etc.); vector and raster graphics editors (CorelDRAW, Adobe Photoshop, etc.); web design tools (Dreamweaver, etc.), typesetting systems (MS Word, LaTeX, OpenOffice)

### Teaching Experience

#### Lecturer

“Semiconducting physics” (2009, Siberian Federal University)

#### Teaching assistant

“Computational methods in physics” (2008, Siberian Federal University)

“Quantum-chemical simulations of crystals properties” (2008, Siberian Federal University)

“Quantum-chemical simulations of structure and properties of solid state” (2014-2018 MIPT)

**Honors, Awards, Fellowships, Memberships of Professional Societies:**

<b>Date</b>	<b>Award</b>
1999	Competition of software projects "Soft-Parade - 99" (nomination "Student"), Krasnoyarsk State University. First degree diploma
2002	VIII Russian Scientific Student Conference on Solid State Physics. Tomsk State University. Second degree diploma.
2003-2004	A participant of Russian Academy of Science – Norilsk Nickel company join program investigation and development hydrogen energy, storage and fuel cells #06-2004
2005	Best student work competition of Krasnoyarsk Regional Fund of a Science. Second degree diploma.
2004-2006	A participant of DFG/RAS program (N 436 RUS 113/785)
2006-2008	RFBR 06-02-16132. The investigations of complex chemical adsorption processes on the surface of carbon nanotubes owing to joint clusters-catalysts of hydrogen decomposition ( <b>participant</b> , project leader: A.S. Fedorov)
2007-2008	The winner of nonprofit organization “Dynasty” competition “Support of PhD students and young scientists”
2008-2010	RFBR 08-02-01096-a. Nanostructures based on the graphene: simulation of structure, electronic and transport properties( <b>participant</b> , project leader: L.A. Chernozatonskii)
2008-2010	RFBR 08-03-00420-a. Nanocomposition materials based on graphene: synthesis and physical-chemical properties ( <b>participant</b> , project leader: A.A. Berlin)
2009-2010	RFBR 09-02-92107. Quantum-chemical and Molecular-dynamics Study of Structure, Properties and Formation Mechanisms of Nanoscale Clusters of Complex Nature ( <b>participant</b> , project leader: S.G. Ovchinnikov)
2011-2013	RFBR 11-02-01453-a. Materials and components for nanoelectronics based on modified graphenes (graphane, diamane, oxide graphene and fluorographene) - modelling of structure and properties ( <b>participant</b> , project leader: L.A. Chernozatonskii)
2012-2013	Research Project of Federal Target Program 14.B37.21.1645. The study of fabrication methods and properties of single-crystal diamond films with nanometer thickness ( <b>project leader</b> )
2013-2014	RFBR 12-02-31261. Investigation of the features of the electronic, elastic and mechanical properties of the materials based on the nanosized diamond clusters ( <b>project leader</b> )
2014-2016	RSF 14-12-01217. Simulation of structure and properties of new nanomaterials based on multilayer transition-metal dichalcogenides and BN-graphene layers ( <b>participant</b> , project leader: L.A. Chernozatonskii)
2015	Award of Academia Europaea for young scientists in physics
2015-2016	Grant of President of Russian Federation for government support of young PhD scientists
2015	Scopus Award Russia 2015 for high scientific activity
2015-2017	NUST MISiS grant to support scientific research implemented under the supervision of the world's leading scientists № K2-2015-033 ( <b>project leader</b> )
2016-2018	RFBR 16-32-60138. Investigation of the features of the properties of the novel 2D materials ( <b>project leader</b> )
2017-2018	NUST MISiS grant to support scientific research implemented under the supervision of the world's leading scientists № K2-2017-001 ( <b>project leader</b> )

**Visiting scientist**

<b>Period</b>	<b>Institution</b>	<b>Head of the group</b>
2006	Humboldt-University of Mathematic, Berlin, Germany	Prof. Jochen W. Brüning
2012	Advanced Science Research Center, Japan Atomic Energy Agency, Japan	Dr. Seiji Sakai
2013	Dresden University of Technology, Dresden, Germany	Prof. Gottard Seifert
2014	Michigan State University, US	Prof. David Tomanek
2015	Advanced Science Research Center, Japan Atomic Energy Agency, Japan	Dr. Seiji Sakai
2017	National Institutes for Quantum and Radiological Science and Technology Quantum Beam Science Research Directorate, Japan	Dr. Seiji Sakai

**Career/Employment**

<b>Period</b>	<b>Position</b>	<b>Institution and place of work</b>
2004/2005	Engineer	Institute of Physics of RAS, Krasnoyarsk, Russia

**Career/Employment**

<b>Period</b>	<b>Position</b>	<b>Institution and place of work</b>
2005/2011	Junior research investigator	Institute of Biochemical Physics of RAS, Moscow, Russia
05.10.2007- 01.12.2010	Students tutor	Siberian Federal University, Krasnoyarsk, Russia
2010/2011	Postdoc research associate	Rice University, Houston, Texas, USA (group of Prof. Boris I Yakobson)
2011/2014	Senior researcher	Technological Institute for Superhard and Novel Carbon Materials, Troitsk, Moscow Region, Russia
2015/up to now	Head of the lab "Laboratory of simulation of new materials"	Technological Institute for Superhard and Novel Carbon Materials, Troitsk, Moscow, Russia
2015/up to now	Leading researcher	National University of Science and Technology MISiS, Moscow, Russia

**Social activity**

<b>Dates</b>	<b>Position</b>	<b>Event</b>
23.04.2008- 24.04.2008	Executive secretary	Interdisciplinary seminar "Measuring and analytical instruments for nanotechnology: modern view and trends of developing", Krasnoyarsk, Russia
24.08.2009- 28.08.2009	Scientific secretary	Workshop "Trends in nanomechanics and nanoengineering", Krasnoyarsk, Russia
13.12.2013	Vice chairman	International seminar "New approaches in materials design", Moscow, Russia
2014-2015	Vice chairman	Regular All-Moscow seminar "Modern theoretical and experimental material science", Moscow, Russia

**Top 10 publications**

1. A.G. Kvashnin, **P.B. Sorokin**, B.I. Yakobson *Flexoelectricity in carbon nanostructures: nanotubes, fullerenes, nanocones* J. Phys. Chem. Lett. **6**, 2740-2744 (2015) (DOI: [10.1021/acs.jpcllett.5b01041](https://doi.org/10.1021/acs.jpcllett.5b01041))
2. J. Hu, X. Liu, C.L. Yue, J.Y. Liu, H.W. Zhu, J.B. He, J. Wei, Z.Q. Mao, L.Yu. Antipina, Z.I. Popov, **P.B. Sorokin**, T.J. Liu, P.W. Adams, S. Radmanesh, L. Spinu, H. Ji and D. Natelson, *Enhanced electron coherence in atomically thin Nb<sub>3</sub>SiTe<sub>6</sub>*, Nature Physics **11**, 6, 471-476 (2015) (DOI: [10.1038/nphys3321](https://doi.org/10.1038/nphys3321))
3. D.G. Kvashnin, **P.B. Sorokin** *Effect of ultrahigh stiffness of defective graphene from atomistic point of view* J. Phys. Chem. Lett. **6**, 12, 2384–2387 (2015)
4. Yu.A. Kvashnina, A.G. Kvashnin, M.Yu. Popov, B.A. Kulnitskiy, I.A. Perezhogin, E.A. Tyukalova, L.A. Chernozatonskii, **P.B. Sorokin**, 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))
5. A.G. Kvashnin, L.A. Chernozatonskii, B.I. Yakobson, **P.B. Sorokin**, *Phase diagram of quasi-two-dimensional carbon*, Nano Letters **14**, 2, pp. 676-681 (2014) (DOI: [10.1021/nl403938g](https://doi.org/10.1021/nl403938g))
6. D.M.Tang., D.G. Kvashnin, S. Najmaei, Y. Bando, K. Kimoto, P. Koskinen, P. Ajayan, B.I. Yakobson, **P.B. Sorokin**, J. Lou, D. Golberg, *Nanomechanical cleavage of molybdenum disulphide atomic layers*, Nature Communications **5**, 3631 (2014) (DOI: [10.1038/ncomms4631](https://doi.org/10.1038/ncomms4631))
7. A.G. Kvashnin, **P.B. Sorokin**, D. Tománek *Graphitic phase of NaCl. Bulk properties and nanoscale stability*. J. Phys. Chem. Lett. **5**, 22, 4014-4019 (2014) (DOI: [10.1021/jz502046f](https://doi.org/10.1021/jz502046f))
8. **P.B. Sorokin**, H. Lee, L. Yu. Antipina, A.K. Singh and B.I. Yakobson *Calcium-decorated carbyne networks as hydrogen storage media* Nano Lett. **11**, 7, 2660–2665 (2011) (DOI: [10.1021/nl200721v](https://doi.org/10.1021/nl200721v))
9. L. Song, L. Ci, H. Lu, **P.B. Sorokin**, C. Jin, J. Ni, A.G. Kvashnin, D.G. Kvashnin, J. Lou, B.I. Yakobson and P.M. Ajayan, *Large scale growth and characterization of atomic hexagonal boron nitride layers* Nano Lett. **10**, 8, 3209-3215 (2010) (DOI: [10.1021/nl1022139](https://doi.org/10.1021/nl1022139))
10. L. A. Chernozatonskii, **P.B. Sorokin** and J. Brüning, *Two-dimensional semiconducting nanostructures based on single graphene sheets with lines of adsorbed hydrogen atoms*, Applied Physics Letters **91**, 183103 (2007) (DOI: [10.1063/1.2800889](https://doi.org/10.1063/1.2800889)) [[arXiv:0709.1015](https://arxiv.org/abs/0709.1015)].

**All publications (in chronological order):****1. Books and reviews**

- 1.1 A.S. Fedorov, P.B. Sorokin, P.V. Avramov, S.G. Ovchinnikov, *Simulation of properties and electronic structure of various carbon and incarbon nanoclusters and its interaction with light elements*, Publishing House of Krasnoyarsk State Polytechnical University, 2006, (multimedia CD-book), ISBN: 5-7692-0817-1 (in Russian)
- 1.2 L.A. Chernozatonskii, P.B. Sorokin, Carbon nanotubes: from fundamental study to nanotechnology in *Carbon investigation – progress and problems*. Ed. T.A. Sladkova. Nauka, Moscow 2007, ISBN: 978-5-02-035594-1, p.154-174 (in Russian).
- 1.3 P.B. Sorokin, L.A. Chernozatonskii. *Graphene-based semiconductor nanostructures* Physics-Uspekhi **56**, 2, pp. 105-122 (2013)
- 1.4 L.A. Chernozatonskii, P.B. Sorokin and A.A. Artukh. *Novel graphene-based nanostructures: physicochemical properties and applications*. Russ. Chem. Rev. **83**, 3, pp. 251-279 (2014)

**2. Contributions to scientific journals**

- 2.1. A.S.Fedorov, P.B.Sorokin *Acceleration of Electronic Structure Calculations for single wall nanotubes* // Bulletin of Krasnoyarsk State University, #1, pp. 55-61 (2004).
- 2.2. P.V.Avramov, P.B.Sorokin, A.S.Fedorov. *Atomic and electronic structure of  $\text{Si}_x\text{C}_{1-x}$  nanotubes* // Bulletin of Krasnoyarsk State University, #4, pp. 139-142 (2005).
- 2.3. A.S. Fedorov, **P.B. Sorokin**. *Method of simplification of calculation of electronic structure calculations for carbon nanotubes*. Physics of the Solid State **47**, 11, 2196-2202 (2005)
- 2.4. A.S. Fedorov, **P.B. Sorokin** *Density and thermodynamics of hydrogen adsorbed inside single-walled carbon nanotubes*. Physics of the Solid State **48**, 2, 402-407 (2006)
- 2.5. **P.B. Sorokin**, A.S. Fedorov, L.A. Chernozatonskii *Structure and properties of BeO-nanotubes*. Physics of the Solid State **48**, 2, pp. 398-401 (2006)
- 2.6. L.A. Chernozatonskii, **P.B. Sorokin**, A.S. Fedorov *Energy and electronic properties of non-carbon nanotubes based on silicon dioxide*. Physics of the Solid State **48**, 10, 2021-2027 (2006)
- 2.7. L.A. Chernozatonskii, **P.B. Sorokin**, E.E. Belova, J. Brünig, A.S. Fedorov *Metal–semiconductor (semimetal) superlattices on a graphite sheet with vacancies*. JETP Letters, **84**, 3, 115-118 (2006)
- 2.8. L.A. Chernozatonskii, V.I. Artyukhov, **P.B. Sorokin**. *Silica nanotube multi-terminal junctions as a coating for carbon nanotube junctions*. Phys. Rev. B **74**, 045402 (2006)
- 2.9. P.V. Avramov, **P.B. Sorokin**, A.S. Fedorov, D.G. Fedorov, Y. Maeda. *Bandgap unification of partially Si-substituted single wall carbon nanotubes*. Phys. Rev. B **74**, 245417 (2006)
- 2.10. P.V. Avramov, A.A. Kuzubov, A.S. Fedorov, **P.B. Sorokin**, F.N. Tomilin, Y. Maeda. *Density-functional theory study of the electronic structure of thin Si/SiO<sub>2</sub> quantum nanodots and nanowires*. Phys. Rev. B **75**, 205427 (2007)
- 2.11. L.A. Chernozatonskii, P.B. Sorokin, E.E. Belova, J. Brünig, A.S. Fedorov. *Superlattices consisting of “lines” of adsorbed pairs of hydrogen atoms on graphene*. JETP Lett. **85**, 1, 77-81 (2007)
- 2.12. P.V. Avramov, L.A. Chernozatonskii, **P.B. Sorokin**, M.S. Gordon *Multiterminal nanowire junctions of silicon: a theoretical prediction of atomic structure and electronic properties*. Nano Lett. **7**, 7, 2063-2067 (2007)
- 2.13. A.S. Fedorov, **P.B. Sorokin**, A.A. Kuzubov *Ab-initio study of hydrogen chemical adsorption on the platinum surface/carbon nanotube join system* Physica Status Solidi B **245**, 8, 1546-1551
- 2.14. L. A. Chernozatonskii, **P.B. Sorokin** and J. Brünig, *Two-dimensional semiconducting nanostructures based on single graphene sheets with lines of adsorbed hydrogen atoms*, Appl. Phys. Lett. **91**, 183103 (2007)
- 2.15. P.V. Avramov, D.G. Fedorov, **P.B. Sorokin**, L.A. Chernozatonskii, M.S. Gordon, *Atomic and electronic structure of new hollow-based symmetric families of silicon nanoclusters*, J. Phys. Chem. C **111**, 18824 (2007).
- 2.16. L.A. Chernozatonskii, **P.B. Sorokin**, B.I. Yakobson, *New boron based barrelenes and tubulens*. JETP Lett. **87**, 489-493 (2008)
- 2.17. **P.B. Sorokin**, P.V. Avramov, A.G. Kvashnin, D.G. Kvashnin, S.G. Ovchinnikov and A.S. Fedorov, *Density functional study of <110> oriented thin silicon nanowires*, Phys. Rev. B **77**, 235417 (2008)
- 2.18. L.A. Chernozatonskii, **P.B. Sorokin** *Electronic superlattices and waveguides based on graphene: structures, properties and applications*, Physica Status Solidi B **245**, 10, 2086-2089 (2008)
- 2.19. P.V. Avramov, **P.B. Sorokin**, D.G. Fedorov, L.A. Chernozatonskii, K. Narumi, S.G. Ovchinnikov and K. Morokuma, *Quantum dots embedded into silicon nanowires effectively partition electron confinement*, J. Appl. Phys. **104**, 054305 (2008)
- 2.20. **P.B. Sorokin**, P.V. Avramov, L.A. Chernozatonskii, D.G. Fedorov, S.G. Ovchinnikov, *Atypical quantum confinement effect in silicon nanowires*, J. Phys. Chem. A **112**, 9955-9964 (2008)

- 2.21. L.A. Chernozatonskii, **P.B. Sorokin**, A.G. Kvashnin, D.G. Kvashnin, *Diamond-like C<sub>2</sub>H nanolayer, diamane: simulation of the structure and properties*, JETP Lett. **90**, 2, 134-138 (2009)
- 2.22. L.A. Chernozatonskii, P.B. Sorokin *Graphene-nanotube ribbon structures: architecture, electronic properties and applications* // ECS Transactions 19, 13, 35-41 (2009)
- 2.23. A.G. Kvashnin, **P.B. Sorokin**, D.G. Kvashnin *Theoretic investigation of mechanical properties of graphene membranes by means of molecular mechanics* // Journal of Siberian Federal University, 2, 4, 426-431 (2009).
- 2.24. L.A. Chernozatonskii, **P.B. Sorokin**, *Nanoengineering structures on graphene with adsorbed hydrogen "lines"* J. Phys. Chem. C **114**, 7, 3225-3229 (2010)
- 2.25. **P.B. Sorokin**, L.A. Chernozatonskii, P.V. Avramov and B.I. Yakobson *Magnesium boride nanotubes: relative stability and atomic and electronic structure* J. Phys. Chem. C **114**, 11, 4852-4856 (2010)
- 2.26. **P.B. Sorokin**, D.G. Kvashnin, A.G. Kvashnin, P.V. Avramov and L.A. Chernozatonskii *Theoretical study of elastic properties of SiC nanowires of different shapes* J. Nanoscience and Nanotechnology **10**, 4992-4997 (2010)
- 2.27. **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**, 5, 2784-2790 (2010)
- 2.28. L. Song, L. Ci, H. Lu, **P.B. Sorokin**, C. Jin, J. Ni, A.G. Kvashnin, D.G. Kvashnin, J. Lou, B.I. Yakobson and P.M. Ajayan, *Large scale growth and characterization of atomic hexagonal boron nitride layers* Nano Lett. **10**, 8, 3209-3215 (2010)
- 2.29. **P.B. Sorokin**, P.V. Avramov, V.A. Demin, L.A. Chernozatonskii *Beta-phase silicon nanowires: structure and electronic properties* JETP Lett. **92**, 5, 352-355 (2010)
- 2.30. A.A. Artyukh, L.A. Chernozatonskii, **P.B. Sorokin**, *Mechanical and electronic properties of carbon nanotube – graphene compounds* Physica Status Solidi (b) **247**, 11-12, 2927-2930 (2010)
- 2.31. L.A. Chernozatonskii, **P.B. Sorokin**, A.A. Kuzubov, B.P. Sorokin, A.G. Kvashnin, D.G. Kvashnin, P.V. Avramov and B.I. Yakobson, *The influence of size effect on the electronic and elastic properties of diamond films with nanometer thickness* J. Phys. Chem. C **115**, 1, 132-136 (2011)
- 2.32. M.A. Ribas, A.K. Singh, **P.B. Sorokin**, and B.I. Yakobson, *Geometrical patterning of nanoroads and quantum dots on fluorinated graphene* Nano Research **4**, 1, 143-152 (2011)
- 2.33. **P.B. Sorokin**, H. Lee, L. Yu. Antipina, A.K. Singh and B.I. Yakobson *Calcium-decorated carbyne networks as hydrogen storage media* Nano Lett. **11**, 7, 2660–2665 (2011)
- 2.34. P.V. Avramov, D.G. Fedorov, **P.B. Sorokin**, S. Sakai, S. Entani, M. Ohtomo, Y. Matsumoto, H. Naramoto, *Intrinsic edge asymmetry in narrow zigzag hexagonal heteroatomic nanoribbons causes their subtle uniform curvature*, J. Phys. Chem. Lett **3**, 2003-2008 (2012)
- 2.35. L.A. Chernozatonskii, B.N. Mavrin and **P.B. Sorokin**, *Determination of ultrathin diamond films by Raman spectroscopy*, Physica Status Solidi B **249**, 8, 1550-1554 (2012)
- 2.36. L.Yu. Antipina, P.V. Avramov, S. Sakai, H. Naramoto, M. Ohtomo, S. Entani, Y. Matsumoto and **P.B. Sorokin**, *High hydrogen-adsorption-rate material based on graphane decorated with alkali metals*, Phys. Rev. B **86**, 085435(7) (2012)
- 2.37. L.A. Chernozatonskii, D.G. Kvashnin, **P.B. Sorokin**, A.G. Kvashnin, J.W. Brüning, *Strong influence of graphane island configurations on the electronic properties of a mixed graphene/graphane superlattice*, J. Phys. Chem. C **116**, 37, 20035-20039 (2012)
- 2.38. D.G. Kvashnin, **P.B. Sorokin**, J.W. Brüning and L.A. Chernozatonskii, *The impact of edges and dopants on the work function of graphene nanostructures. The way to high electronic emission from pure carbon medium*, Appl. Phys. Lett. **102**, 18, 183112(5) (2013).
- 2.39. S. Sakai, Y. Matsumoto, M. Ohtomo, S. Entani, P.V. Avramov, **P.B. Sorokin**, H. Naramoto, *High spin polarization at the Fe/C<sub>60</sub> interface in the Fe-doped C<sub>60</sub> film*, Synthetic Metals **173**, 22-25 (2013)
- 2.40. Yu.A. Kvashnina, A.G. Kvashnin, **P.B. Sorokin**, *Investigation of new superhard carbon allotropes with promising electronic properties*, J. Appl. Phys. **114**, 183708(5) (2013)
- 2.41. A.G. Kvashnin, **P.B. Sorokin**, *Lonsdaleite films with nanometer thickness*, J. Phys. Chem. Lett. **5**, 541-548 (2014)
- 2.42. A.G. Kvashnin, L.A. Chernozatonskii, B.I. Yakobson, **P.B. Sorokin**, *Phase diagram of quasi-two-dimensional carbon*, Nano Lett. **14**, 2, 676-681 (2014)
- 2.43. D.M. Tang., D.G. Kvashnin, S. Najmaei, Y. Bando, K. Kimoto, P. Koskinen, P. Ajayan, B.I. Yakobson, **P.B. Sorokin**, J. Lou, D. Golberg, *Nanomechanical cleavage of molybdenum disulphide atomic layers*, Nature Commun. **5**, 3631(8) (2014)
- 2.44. D.G. Kvashnin, L.Yu. Antipina, **P.B. Sorokin**, R. Tenne, D. Golberg, *Theoretical aspects of WS<sub>2</sub> nanotube chemical unzipping*, Nanoscale **6**, 8400-8404 (2014)
- 2.45. Y. Sun, A.G. Kvashnin, **P.B. Sorokin**, B.I. Yakobson, W.E. Billups *Radiation-induced nucleation of diamonds from amorphous carbon. Effect of hydrogen*, J. Phys. Chem. Lett. **5**, 11, 1924-1928 (2014)

- 2.46. A.G. Kvashnin, **P.B. Sorokin**, D. Tománek *Graphitic phase of NaCl. Bulk properties and nanoscale stability*. J. Phys. Chem. Lett. **5**, 22, 4014-4019 (2014)
- 2.47. A.V. Krasheninnikov, N. Berseneva, D.G. Kvashnin, J. Enkovaara, T. Björkman, **P. Sorokin**, D. Shtansky, R.M. Nieminen, D. Golberg *Towards stronger Al-BN nanotube composite materials: getting insight into bonding at the Al/BN interface from first-principles calculations* J. Phys. Chem. C **118**, 46, 26894-26901 (2014)
- 2.48. **P.B. Sorokin**, A.G. Kvashnin, Z. Zhu, D. Tománek *Spontaneous graphitization of ultrathin cubic structures: A computational study* Nano Lett. **14**, 12, 7126-7130 (2014)
- 2.49. L.Yu. Antipina, **P.B. Sorokin**, *Converting chemically functionalized few-layer graphene to diamond films: A computational study*. J. Phys. Chem. C **119**, 2828-2836 (2015)
- 2.50. D.G. Kvashnin, P. Vancsó, L.Yu. Antipina, G.I. Márk, L.P. Biró, **P.B. Sorokin** and L.A. Chernozatonskii *Bilayered graphene nanostructures with periodically arranged hexagonal holes*. Nano Research **8**, 4, 1250-1258 (2015)
- 2.51. S. Entani, L.Yu. Antipina, P.V. Avramov, M. Ohtomo, Y. Matsumoto, N. Hirao, I. Shimoyama, H. Naramoto, Y. Baba, **P.B. Sorokin** and S. Sakai, *Graphene/sapphire heterostructure: contracted interlayer distance and hole-doping through electrostatic interactions*, Nano Research **8**, 5, 1535-1545 (2015)
- 2.52. Yu.A. Kvashnina, A.G. Kvashnin, M.Yu. Popov, B.A. Kulnitskiy, I.A. Perezhogin, E.A. Tyukalova, L.A. Chernozatonskii, **P.B. Sorokin**, V.D. Blank, *Toward the ultra-incompressible carbon materials. Computational simulation and experimental observation*, J. Phys. Chem. Lett. **6**, 2147-2152 (2015)
- 2.53. J. Hu, X. Liu, C.L. Yue, J.Y. Liu, H.W. Zhu, J.B. He, J. Wei, Z.Q. Mao, L.Yu. Antipina, Z.I. Popov, **P.B. Sorokin**, T.J. Liu, P.W. Adams, S. Radmanesh, L. Spinu, H. Ji and D. Natelson, *Enhanced electron coherence in atomically thin Nb<sub>3</sub>SiTe<sub>6</sub>*, Nature Physics **11**, 6, 471-476 (2015)
- 2.54. D.G. Kvashnin, **P.B. Sorokin** *Effect of ultrahigh stiffness of defective graphene from atomistic point of view* J. Phys. Chem. Lett. **6**, 12, 2384-2387 (2015)
- 2.55. D.G. Kvashnin, **P.B. Sorokin**, D. Shtansky, D. Golberg, A.V. Krasheninnikov, *Line and rotational defects in boron-nitrene: structure, energetics, and dependence on mechanical strain from first-principles calculations*, Phys. Status Solidi B **252**, 1725-1730 (2015)
- 2.56. A.G. Kvashnin, **P.B. Sorokin**, B.I. Yakobson *Flexoelectricity in carbon nanostructures: nanotubes, fullerenes, nanocones* J. Phys. Chem. Lett. **6**, 2740-2744 (2015)
- 2.57. C. Zhang, Z. Xu, D.G. Kvashnin, Y. Bando, **P.B. Sorokin**, D. Golberg. *Opto-mechano-electrical tripling in ZnO nanowires probed by photocurrent spectroscopy in a high-resolution transmission electron microscope* Appl. Phys. Lett. **107**, 091103(4) (2015)
- 2.58. T.R.J. Bollman, L.Yu. Antipina, M. Reichling, **P.B. Sorokin** *Hole doping of mechanically exfoliated graphene by confined hydration layers* Nano Research **8**, 9, 3020-3026 (2015)
- 2.59. S. V. Erohin, **P. B. Sorokin** *Elastic properties of nanopolycrystalline diamond: The nature of ultrahigh stiffness* Appl. Phys. Lett. **107**, 121904(3) (2015)
- 2.60. P. Avramov, V. Demin, M. Luo, C.H. Choi, **P.B. Sorokin**, B. Yakobson and L. Chernozatonskii *Translation Symmetry Breakdown in Low-Dimensional Lattices of Pentagonal Rings* J. Phys. Chem. Lett. **6**, 4525-4531 (2015)
- 2.61. D.G. Kvashnin, **P.B. Sorokin**, G. Seifert, L.A. Chernozatonskii *MoS<sub>2</sub> decoration by Mo-atoms and MoS<sub>2</sub>-Mo-graphene heterostructure: a theoretical study* Phys. Chem. Chem. Phys. **17**, 28770-28773 (2015)
- 2.62. P.V. Avramov, **P.B. Sorokin**, S. Sakai, M. Ohtomo, S. Entani, Y. Matsumoto, H. Naramoto. *Prospects of spin catalysis on spin-polarized graphene heterostructures* Aust. J. Chem. **69**, 7, 753-758 (2015).
- 2.63. D.G. Kvashnin, A.V. Krasheninnikov, D. Shtansky, **P.B. Sorokin**, D. Golberg. *Nanostructured BN – Mg Composite: Features of Interface Bonding and Mechanical Properties* Phys. Chem. Chem. Phys. **18**, 965-969 (2016)
- 2.64. K.L. Firestein, D.G. Kvashnin, A.N. Sheveyko, I.V. Sukhorukova, A.M. Kovalskii, A.T. Matveev, O.I. Lebedev, **P.B. Sorokin**, D. Golberg, D.V. Shtansky *Structural analysis and atomic simulation of Ag/BN nanoparticle hybrids obtained by Ag ion implantation* Materials & Design **98**, 167-173 (2016)
- 2.65. 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)
- 2.66. L.A. Chernozatonskii, A.G. Kvashnin, **P.B. Sorokin** *Heterostructures based on graphene and MoS<sub>2</sub> layers decorated by C<sub>60</sub> fullerenes* Nanotechnology **27**, 36, 365201 (2016)
- 2.67. S. Entani, M. Mizuguchi, H. Watanabe, L.Yu. Antipina, **P.B. Sorokin**, P.V. Avramov, H. Naramoto, S. Sakai *Effective fluorination of single-layer graphene by high-energy ion irradiation through a LiF overlayer* RSC Advances **6**, 68525-68529 (2016)
- 2.68. S. Sakai, S. Majumdar, Z.I. Popov, P.V. Avramov, S. Entani, Y. Hasegawa, Y. Yamada, H. Huhtinen, H. Naramoto, **P.B. Sorokin**, Y. Yamauchi *Proximity-induced spin polarization of graphene in contact with half-metallic manganite* ACS Nano **10**, 8, 7532-7541 (2016)

- 2.69. E.Y. Pashkin, A.M. Pankov, B.A. Kulnitskiy, I.A. Perezhogin, A.R. Karaeva, V.Z. Mordkovich, M.Y. Popov, **P.B. Sorokin**, V.D. Blank *The unexpected stability of multiwall nanotubes under high pressure and shear deformation* Appl. Phys. Lett. **109**, 081904(3) (2016)
- 2.70. L.Yu. Antipina, A.G. Kvashnin, **P.B. Sorokin**, L.A. Chernozatonskii *The possible formation of magnetic FeS<sub>2</sub> phase in two-dimensional MoS<sub>2</sub> matrix* Phys. Chem. Chem. Phys. **18**, 26956-26959 (2016)
- 2.71. C. Zhang, O. Cretu, D.G. Kvashnin, N. Kawamoto, M. Mitome, X. Wang, Y. Bando, **P.B. Sorokin**, D. Golberg *Statistically analyzed photoresponse of elastically bent CdS nanowires probed by light-compatible in situ high-resolution TEM* Nano Letters **16**, 6008-6013 (2016)
- 2.72. X. Liu, J. Liu, L.Yu. Antipina, J. Hu, C. Yue, A.M. Sanchez, **P.B. Sorokin**, Z. Mao, J. Wei *Direct fabrication of functional ultrathin single-crystal nanowires from quasi-one-dimensional Van der Waals crystals* Nano Letters **16**, 6188-6195 (2016)
- 2.73. D.G. Kvashnin, M. Ghorbani-Asl, D.V. Shtansky, D.V. Golberg, A.V. Krashennnikov, **P.B. Sorokin** *Mechanical properties and current-carrying capacity of Al reinforced with graphene/BN nanoribbons: a computational study* Nanoscale **8**, 20080-20089 (2016)
- 2.74. Z.I. Popov, N.S. Mikhaleva, M.A. Visotin, A.A. Kuzubov, S. Entani, H. Naramoto, S. Sakai, **P.B. Sorokin**, P.V. Avramov *Electronic Structure and Spin States of 2D graphene/VX<sub>2</sub> (X=S,Se) Heterostructures* Phys. Chem. Chem. Phys. **18**, 33047-33052 (2016)
- 2.75. A.V. Telichko, S.V. Erohin, G.M. Kvashnin, **P.B. Sorokin**, B.P. Sorokin, V.D. Blank *Diamond's third order elastic constants: ab initio calculations and experimental investigation* J. Mater. Sci. **52**, 3447-3456 (2017)
- 2.76. M. Annenkov, V. Blank, B. Kulnitskiy, K. Larionov, D. Ovsyannikov, I. Perezhogin, M. Popov, **P. Sorokin** *Boron carbide nanoparticles for high-hardness ceramics: crystal lattice defects after treatment in a planetary ball mill* J. Eur. Cer. Soc. **37**, 4, 1349-1353 (2017)
- 2.77. Y. Xue, P. Dai, M. Zhou, X. Wang, A. Pakdel, C. Zhang, Q. Weng, T. Takei, X. Fu, Z.I. Popov, **P.B. Sorokin**, C. Tang, K. Shimamura, Y. Bando, D. Golberg *Multifunctional Superelastic Foam-Like Boron Nitride Nanotubular Cellular-Network Architectures* ACS Nano **11**, 1, P. 558-568 (2017)
- 2.78. Y.A. Kvashnina, A.G. Kvashnin, L.A. Chernozatonskii, **P.B. Sorokin** *Fullerite-based nanocomposites with ultrahigh stiffness. theoretical investigation* Carbon **115**, P. 546-549 (2017)
- 2.79. P. Avramov, A.A. Kuzubov, A.V. Kuklin, H. Lee, E.A. Kovaleva, S. Sakai, S. Entani, H. Naramoto, **P.B. Sorokin** *Theoretical Investigation of the Interfaces and Mechanisms of Induced Spin Polarization of 1D Narrow Zigzag Graphene- and h-BN Nanoribbons on a SrO-Terminated LSMO(001) Surface* J. Phys. Chem. A **121**, 3, 680-689 (2017)
- 2.80. 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)
- 2.81. E. Kano, D.G. Kvashnin, S. Sakai, L.A. Chernozatonskii, **P.B. Sorokin**, A. Hashimoto, M. Takeguchi *One-atom-thick 2D copper oxide clusters on graphene* Nanoscale **9**, 3980-3985 (2017)
- 2.82. Y.A. Kvashnina, D.G. Kvashnin, A.G. Kvashnin, **P.B. Sorokin** *New allotropic forms of carbon based on C<sub>60</sub> and C<sub>20</sub> fullerenes with specific mechanical characteristics* JETP Lett. **105**, 7, 419-425 (2017)
- 2.83. A.V. Kuklin, A.A. Kuzubov, E.A. Kovaleva, H. Lee, **P. Sorokin**, S. Sakai, S. Entani, H. Naramoto, P. Avramov, *The direct exchange mechanism of induced spin polarization of low-dimensional pi-conjugated carbon- and h-BN fragments at LSMO(001) MnO-terminated interfaces* J. Magnetism and Magnetic Mat. **440**, 23-29 (2017)
- 2.84. A.G. Kvashnin, P.V. Avramov, S. Sakai, Y.S. Netchaev, **P.B. Sorokin** *Estimation of graphene surface stability against the adsorption of environmental and technological chemical agents* Physica Status Solidi B **254**, 6, 1600702 (2017)
- 2.85. Q. Weng, D.G. Kvashnin, O. Cretu, M. Zhou, C. Zhang, D.M. Tang, **P.B. Sorokin**, Y. Bando, D. Golberg *Optical, electronic and magnetic property tuning of boron nitride nanosheets with oxygen doping and functionalization* Adv. Mater. **29**, 28, 1700695 (2017)
- 2.86. E.A. Kovaleva, A.A. Kuzubov, P.V. Avramov, A.S. Kholobina, A.V. Kuklin, F.N. Tomilin, **P.B. Sorokin** *A key role of tensile strain and surface termination in formation and properties of La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> composites with carbon nanotubes* Comp. Mat. Sci. **139**, 125-131 (2017)
- 2.87. 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)
- 2.88. A.G. Kvashnin, P.V. Avramov, D.G. Kvashnin, L.A. Chernozatonskii, **P.B. Sorokin** *The features of electronic, mechanical and electromechanical properties of fluorinated diamond films of nanometer thickness* J. Phys. Chem. C. **121**, 51, 28484-28489 (2017)
- 2.89. A. Konopatsky, K.L. Firestein, D.V. Leybo, Z.I. Popov, K.V. Larionov, A.E. Steinman, A.M. Kovalskii, A.T. Matveev, A. Manakhov, **P.B. Sorokin**, D. Golberg, D.V. Shtansky *BN Nanoparticle/Ag Hybrids with Enhanced Catalytic Activity: Theory and Experiments* Catal. Sci. Technol. **8**, 1652-1662 (2018).



- 2.90. A.E. Steinman, C. Shakti, K.L. Firestein, D.G. Kvashnin, A.M. Kovalskii, A.T. Matveev, **P.B. Sorokin**, D. Golberg, D.V. Shtansky *Al-based composites reinforced with AlB<sub>2</sub>, AlN and BN Phases: experimental and theoretical studies* *Materials & Design* **141**, 88-98 (2018).
- 2.91. T. Watanabe, Y. Yamada, A. Koide, S. Entani, S. Li, Z.I. Popov, **P.B. Sorokin**, H. Naramoto, M. Sasaki, K. Amemiya, S. Sakai *Interface-induced perpendicular magnetic anisotropy of Co nanoparticles on single-layer h-BN/Pt(111)* *Appl. Phys. Lett.* **112**, 2, 022407 (2018).
- 2.92. A.P. Tsapenko, A.E. Goldt, E. Shulga, Z.I. Popov, K.I. Maslakov, A.S. Anisimov, **P.B. Sorokin**, A.G. Nasibulin *Highly conductive and transparent films of HAuCl<sub>4</sub>-doped single-walled carbon nanotubes for flexible applications* *Carbon* **130**, 448-457 (2018)
- 2.93. V.D. Blank, V.D. Churkin, B.A. Kulnitskiy, I.A. Perezhogin, A.N. Kirichenko, S.V. Erohin, **P.B. Sorokin** and M.Y. Popov *Pressure-Induced Transformation of Graphite and Diamond to Onions Crystals* **8**, 68 (2018)
- 2.94. V.D. Blank, V.D. Churkin, B.A. Kulnitskiy, I.A. Perezhogin, A.N. Kirichenko, V.N. Denisov, S.V. Erohin, **P.B. Sorokin** and M.Y. Popov *Phase diagram of carbon and the factors limiting the quantity and size of natural diamonds* *Nanotechnology* **29**, 11, 115603 (2018)
- 2.95. M. Zhou, Q. Weng, Z.I. Popov, Y. Yang, L.Yu. Antipina, **P.B. Sorokin**, X. Wang, Y. Bando, D. Golberg *Construction of Polarized Carbon-Nickel Catalytic Surfaces for Potent, Durable, and Economic Hydrogen Evolution Reactions* *ACS Nano* **12**, 5, 4148-4155 (2018)
- 2.96. S. Sakai, S.V. Erohin, Z.I. Popov, S. Haku, T. Watanabe, Y. Yamada, S. Entani, S. Li, P.V. Avramov, H. Naramoto, K. Ando, **P.B. Sorokin**, Y. Yamauchi *Dirac cone spin polarization of graphene by magnetic insulator proximity effect probed with outermost surface spin spectroscopy* *Advanced Functional Materials* **28**, 1800462 (2018)
- 2.97. K. Faerstein, D.G. Kvashnin, A.M. Kovalskii, Z.I. Popov, **P.B. Sorokin**, D. Golberg, D. Shtansky *Compressive Properties of Hollow BN Nanoparticles: Theoretical Modeling and Testing in a High-Resolution Transmission Electron Microscope* *Nanoscale* **10**, 8099-8105 (2018)
- 2.98. K.V. Larionov, Z.I. Popov, M.A. Vysotin, D.G. Kvashnin, **P.B. Sorokin** *Study of the New Two-Dimensional Compound CoC* *JETP Lett.* (2018)
- 2.99. J.F.S. Fernando, M.P. Shortell, K.L. Firestein, C. Zhang, K. Larionov, Z.I. Popov, **P.B. Sorokin**, L. Bourgeois, E.R. Waclawik, D. Golberg *Photocatalysis with Pt-Au-ZnO and Au-ZnO Hybrids: Effect of Charge Accumulation and Discharge Properties of Metal Nanoparticles* *Langmuir* **34**, 25, 7334-7345 (2018)
- 2.100. N.A. Nebogatikova, I.V. Antonova, S.V. Erohin, D.G. Kvashnin, A. Olejniczak, V.A. Volodin, A.V. Skuratov, A.V. Krashennnikov, **P.B. Sorokin**, L.A. Chernozatonskii *Nanostructuring few-layer graphene films by swift heavy ions for electronic application: tuning of electronic and transport properties* *Nanoscale* **10**, 14499-14509 (2018)
- 2.101. K.V. Larionov, D.G. Kvashnin, **P.B. Sorokin** *2D FeO: a New Member in 2D Metal Oxide Family* *J. Phys. Chem. C* **122**, 30, 17389-17394 (2018)
- 2.102. D.M. Tang, D.G. Kvashnin, O. Cretu, Y. Nemoto, F. Uesugi, M. Takeguchi, X. Zhou, F.C. Hsia, C. Liu, **P.B. Sorokin**, N. Kawamoto, M. Mitome, H.M. Cheng, D. Golberg, Y. Bando *Chirality transitions and transport properties of individual few-walled carbon nanotubes as revealed by in situ TEM probing* *Ultramicroscopy* (2018)