Name	Alexey
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Date of birth	18 Nov. 1984
Marital status	Married, one child
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Work experience

2010-present	Research fellow	Moscow State University, Faculty of Biology, Department of Bioengineering; focus on computer simulations of bio and nano structures
2010	Scientific Co-ordinator	Russian Technology Platform "Supercomputers and high performance computing"
2008-2010	Leading engineer	Moscow State University, Faculty of Biology, Department of Bioengineering; focus on IT infrastructure for computer simulations
2009-2011	Research fellow	University of Ulm, Institute of Polymer Science, director Prof. A.R. Khokhlov, Ulm, Germany
2006-2008	Teacher	School N1326/Lyceum 1586, subjects: computer modeling (10-11 grades), computer methods in biology and physics (7-9 grades)

Education

2011	Dr. Rer. Nat. (PHD)	University of Ulm, thesis title "Computer simulations of self-assembling nanofibers from thiophene-peptide oligomers", supervisor Prof. A.R. Khokhlov
2010	PHD degree (physics and mathematics)	Moscow State University, thesis title "Computer simulations and statistical analysis of self-organizing molecular structures based on peptides", supervisor Prof. A.R. Khokhlov
2007-2010	PHD student	Moscow State University, Faculty of Physics, Chair of Physics of Polymers and Crystals, supervisor Prof. A.R. Khokhlov
2007-2008		"Innovation Studio" Entrepreneurship Program at Moscow State University
2001-2007	MSc	Moscow State M.V. Lomonosov University, Faculty of Physics, Chair of Physics of Polymers and Crystals, diploma with excellence (GPA 5.0, max 5.0), Master Thesis "Study of hydration and adsorption of amino acid side chains vie MD simulations" (selected as best master thesis on chair)
2002-2005		Russian-German Institute of Science and Culture at MSU
1991-2001		Moscow comprehensive school No. 1260 with profound study of English. School-leaving certificate with excellence (GPA 5.0, max 5.0)

Honors and awards

2008	BioCamp 2008, Novartis International Biotechnology Leadership Camp, Hong Kong: leader of the best Best Performing Team, 2nd Runner Up Best Performing Student
2008	Laureate UMNIK Program, Foundation for Assistance to Small Innovative Enterprises (FASIE)
2008	Russian Innovation Contest, participant of the 2nd round
2005	Scholarship of Vladimir Potanin Fund
2005	Scholarship "Grant of Moscow"

Research grants

2012	Russian Foundation for Basic Research young scientist grant №12-04-31942 "Supercomputer simulations of structure and dynamics of nucleosomes"
2012	Joint grant of Centre national de la recherche scientifique and Moscow State University "Modulation of the function of voltage-gated potassium channels: Molecular Dynamics simulations" (with Dr. Mounir Tarek, Nancy University)

Student co-supervision

2011, master thesis, Moscow State University, M.A. Kasimova "Molecular dynamics study of ion current through potassium KcsA ion channel"
2010, master thesis, Moscow State University, M.E. Bozdaganyan "Molecular dynamics simulations of C60 and C3 interactions with biological membranes"
2010, master thesis, Moscow State University, F.S. Orekhov "Calculation of adsorption spectra of bacteriorhodopsin using QM/MM techniques"

Qualification degrees and certificates

- Second qualification degree as teacher, since 2007, Lyceum 1586
- German language certificate DSH, level 3.

Language Skills

Russian (native), English (fluent), German (fluent, DSH-3), French (limited)

Research skills

Methods. **Computer simulations of soft matter and biological systems: MD simulations,** free energy estimation methods (FEP, BAR, TI), docking, macromolecular docking, dissipative particle dynamics, **quantum chemistry (HF, DFT, spectral calculations, electron transfer), statistical analysis, good understanding of statistical physics.**
Objects. **Biological membranes, ion channels, nano particles, photosensory proteins, amyloid fibers, polymer bioconjugates.**
Software. **Open source MD codes (LAMMPS,** GROMACS, AMBER, NAMD, Tinker), HyperChem, ChemOffice, Accelrys Materials Studio, Gaussian, visualization (VMD, 3dsMAX, POV-Ray, Tachyon), AutoCAD.

IT skills

Assembly and Management of High Performance Linux Computer Clusters (links to clusters assembled and administered by me: http://aldan2.physik.uni-ulm.de, http://biosim.moldyn.org), Linux (cluster and server administration level), Bash scripting, PERL, C/C++, MS Visual C++, Fortran, IP networks, MPI (compilation on supercomputing facilities), MySQL, web development on CMS (DRUPAL, group web-site developed by me http://www.molsim.org).

Research interests

- Function of ion channels as potential drug targets studied by MD simulations.
- Molecular dynamics simulations of polymers and biopolymers. Basic principles and free energy calculations.
- Self-organization of polymer-bioconjugates and amyloid-like structures. Design of conductive bioinspired nanowires.
- Spectral properties of rhodopsin proteins and their mutant forms studied via QM/MM calculations.
- Membrane simulations and interaction of nano particles with biological membranes. Atomistic and coarse-grain simulations.
- Structure and function of nucleosomes and elongation complexes

Selected publications

1. Orekhov F.S., Shaytan A.K., Shaitan K.V. Calculation of spectral shifts of the mutants of bacteriorhodopsin by QM/MM methods. Biofizika. 2012, 57(2), pp. 221-31.
2. Shaytan A.K., Schillinger E.-K., Mena-Osteritz E., Schmid S., Khalatur P.G., Bäuerle P., Khokhlov A.R. Self-organizing bioinspired oligothiophene-oligopeptide hybrids. // Beilstein Journal of Nanotechnology, 2011, 2, 525-544, DOI: 10.3762/bjnano.2.57
3. Shaytan A. K., Schillinger E.-K., Khalatur P. G., Mena-Osteriz E., Hentschel J., Boerner H.G., Baeuerle P, Khokhlov A. R., Self-assembling Nanofibers from Thiophene-Peptide Diblock Oligomers: a Combined Experimental and Computer Simulations Study // ACSNano, 2011, DOI: 10.1021/nn2011943
4. Shaytan A. K., Khokhlov A. R., Khalatur P. G. Large-scale atomistic simulation of a nanosized fibril formed by thiophene-peptide “molecular chimeras” // Soft Matter, 2010, 6, pp 1453—1461, DOI: 10.1039/b918562c
5. Shaytan A.K., Ivanov V.A., Shaitan K.V., Khokhlov A.R. "Free energy profiles of amino acid side chain analogs near water-vapor interface obtained via MD simulations", // Journal of Computational Chemistry, 2010, 31(1), pp 204-216, DOI: 10.1002/jcc.21267
6. Shaytan A.K, Shaitan K.V., Khokhlov A.R. “Solvent Accessible Surface Area of Amino Acid Residues in Globular Proteins: Correlation of Apparent Transfer Free Energies with Experimental Hydrophobicity Scales. // Biomacromolecules, 2009, 10 (5), pp 1224–1237, DOI: 10.1021/bm8015169
7. Shaitan K.V., Tourleigh Ye.V., Golik D.N., Tereshkina K.B., Levtsova O.V., Fedik I.V., Shaytan A.K., Li A., Kirpichnikov M.P. "Dynamics and molecular design of bio- and nanostructures" // Rossiyskiy Khimicheskiy Zhurnal (in Russian), 2006, 50 (2), 53–65
8. Shaitan K.V., Tourleigh Ye.V., Golik D.N., Tereshkina K.B., Levtsova O.V., Fedik I.V., Shaytan A.K., Kirpichnikov M.P. "Nonequilibrium molecular dynamics of nanostructures including biological ones” // Khimicheskaya Fizika (in Russian), 2006, 25 (9), 31–48
9. Shaitan K.V., Tourleigh Ye.V., Golik D.N., Tereshkina K.B., Levtsova O.V., Fedik I.V., Shaytan A.K., Kirpichnikov M.P., «Molecular dynamics and design of bio- and nanostructures», Vestnik Biotechnologii (in Russian), 2005, 1 (1), pp. 66-78

Talks

- 22 Aug 2012 – IV Russian Biophysical Meeting, N. Novgorod, “Computer simulations of amyloid-like fibrils”
- 27 Mar 2012 – Polymer Blends 2012, San Sebastian, invited talk, “Design of block copolymer nanostructures in the bulk and in thin films”, A.K. Shaytan, A.R. Khokhlov
- 30 Nov 2011 – University of Marburg, “Computer Simulations of Self-assembling Nanofibers from Thiophene-Peptide Oligomers”

References available on request