Aleksey Vishnyakov

Leading Research Scientist

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Primary expertise: physical chemistry of nanostructured systems, molecular modeling techniques

Other research topics: characterization and modeling of nanostructured materials, dynamics of macromolecules, phase transitions in lipid layers

Education and training:

Ph. D. in Chemistry, (к. х. н.) St. Petersburg State University 1998
(molecular simulation of phase equilibria in nanoporous materials
advisor: Dr. E.M. Piotrovskaya)

Specialist in Computer Science (Программное обеспечение вычислительной техники), St. Petersburg State University 1995

visiting student
Technical University of Berlin 1995
(modelling of ethylene polymerisation using equations of state,
advisor: Prof. Wolfgang D Arlt)

visiting student, 1998
MEMPHYS Center of Biomembrane Physics, Technical University of Denmark
(advisor Prof Ole G Mouritsen)

- Performed simulations of phase transitions in phospholipid membranes

visiting student, 1998
Arrhenius Laboratory, Stockholm University. (advisor Prof. Aatto Laaksonen).

- developed molecular forcefields, examined solvation and dynamics of disaccharides in complex solutions

Research:

Leading Research Scientist, Inst. of Solution Chemistry RAS Mar **2023-**
Ivanovo, Russia

Moscow State Univ. (Dept. Physics) Mar **2023**-

Leading Research Scientist, Thermal Petrophysics Inc. Oct **2021-**Feb **2023**
Moscow, Russia

Associate Professor, Skolkovo Inst. Sci. & Technol. **2021-2022**
Center for Petroleum Engineering

Associate Professor, Skolkovo Inst Sci. & Technol., **2018-2021**
Center for computational and data-intensive science and engineering

Associate research professor, Dept. Chemical &
Biochemical Engineering Rutgers Univ. **2012-2017**
Assistant research professor **2006-2011**

- directed nanomaterials computational laboratory, mentored and consulted students on computational problems.
- developed a simulation technique for mesoscale modelling of nanostructured polyelectrolytes
- developed a new simulation technique for modelling nucleation in multicomponent systems
- developed forcefields and explored structure and dynamics of block ionomers
- advised graduate students (list attached)
- wrote research proposals to US agencies and companies (see funding list)

staff scientist, TRI/Princeton **1999-2006**

- developed simulation techniques for nanostructured fluids
- developed forcefields and explored structure and dynamics of Nafion polyelectrolyte membranes
- explored nucleation and phase transitions in nanoconfinements
- simulation results were incorporated into commercial software/equipment for nanomaterials characterization by Quantachrome Inc.
- wrote research proposals to US agencies and companies
- carried out programming in Fortran and C

Teaching:

Skolkovo Inst Sci&Techn. Course development& teaching Thermodynamics and transport at nanoscale (new: 2019-2022) Soft condensed matter (newly developed: 2020,2022) Parallel computing in mathematical modeling and data-intensive applications (co-developed 2020-2022) Molecular Simulation Techniques (short winter course: 2021, 2022)	2019-2023
Instructor, Rutgers University Co-developed and taught a new graduate course “Fundamentals of Nanoscale Thermodynamics and Transport”.	2008-2014

Invited Instructor Summer School on Nanoscale Thermodynamics and Molecular Simulations, Nanjing University, PR China	2012
Adjunct Professor *Department of Chemistry , Brookdale College* NJ, USA (Chem106 "Chemistry and Society")	2010-2011
Teaching Assistant, Statistical Mechanics undergraduate course, St. Petersburg State University. (Evaluated quizzes and home works, occasionally gave lectures)	1996

Academic Awards and Fellowships:

- Nordic Council of Ministers Fellowship 1998
- International Science Foundation Graduate Student 1997
- Honorary Scholarship of the President of Russian Federation (for graduate students) 1996
- Special distinction for the best master thesis by the State Graduation Examination Commission 1995

Synergetic activities:

Coordinator of seminar "Physics- and data-driven modeling on micro- and nanoscale" (SkT and outside presenters, including guestst from the US, PRC and Germany; online during the Covid restrictions, we are preparing for restart in offline-hybrid mode Sep 22)
Organizer and chair: "Molecular and mesoscale simulations for oil & gas" workshop, Jan 2020
Organized, scheduled and chaired sessions at the annual meetings of American Institute of Chemical Engineers:

- *Metal-Organic Adsorption Materials*, AIChE Meeting, San Francisco, November 16-21, 2003.
- *New Developments in Adsorption and Ion Exchange.* AIChE Meeting, Indianopolis, November 3-8, 2002.

Assistant organizer of the International Workshop "Characterization of Porous Materials: from Angstroms to millimeters V, VI, VII" (2006-2015)
Member of programming Committee for AICHE section 2E "Adsorption and ion exchange" 2009-2017
Referee: ACS PRF grant proposals, NWO computational facilities proposals, Glance into the future awards for young scientists

Trainees: PhD students, Master students, Postdocs, Research Engineers

Service:

Member of Skoltech Research and Innovations committee, 2021-2022
Skoltech Teaching Assistant policy group, 2019-2020
Member of Educational Committee, Data & Computational Science, 2018-2021

Member of FACIP committee at Rutgers Dept Chem Eng (2015-2016, 2016-2017)
Other service: Faculty Advisor to Rutgers Undergraduate Chess Club, tournament director, team captain in NJ chess league

Inventions:

J. Landers, A. V. Neimark, T. Asefa, A. Vishnyakov, A. Goswami, J. C. Ortiz, Multicatalyst Polyelectrolyte Membranes and Materials and Methods Utilizing the Same. US Patent 10,722,743 B2 (2020).

Invited seminars & conference presentations (last 3 yrs):

Nanoparticle interactions with soft surfaces studies with coarse-grained simulations. Krestov Inst. of Solutions Chemistry, RAS. Feb 2023

Carbopol – water interafces: dissipatice particle dynamics study. Moscow State Univ., Dept. physics. Oct 2022

Publications (H-index 39 GS, 36 Scopus):

[1] *Beloborodov D.,Vishnyakov A.* Molecular Dynamics of Nanodroplet Coalescence in Quasi-Saturated Vapor // Fluids. 2023. V. 8 № 2. P. 77.

[2] *Akeweje E., Vanovskiy V.,Vishnyakov A.* Surrogate models of hydrogen oxidation kinetics based on deep learning (Суррогатные модели кинетики горения водорода на основе глубокого обучения) // Theor. Found. Chem. Eng. (Теор. Осн. Хим. Техн.). 2023. V. 57 № 2. P. 1-9.

[3] *Kopanichuk I.V., Vishnyakov A.M., Sizova A.A., Sizov V.V., Vanin A.A.,Brodskaya E.N.* Influence of Surfactants on Hydrocarbon Mobility in Narrow Pores in the Presence of Water (Влияние поверхностно-активных веществ на подвижность углеводорода в узких порах в присутствии воды) // Colloid J. (Коллоидный ж-л). 2022. V. 84 № 4. P. 477-484.

[4] *Kopanichuk I.V., Santo K.P.,Vishnyakov A.M.* The effects of multiparticle interactions on the aggregation of asphaltenes // Colloids and Surfaces a-Physicochemical and Engineering Aspects. 2022. V. 636 №. P. 10.

[5] *Kopanichuk I., Scerbacova A., Ivanova A., Cheremisin A.,Vishnyakov A.* The effect of the molecular structure of alkyl ether carboxylate surfactants on the oil–water interfacial tension // Journal of Molecular Liquids. 2022. V. 360 №. P. 119525.

[6] *Faria B.F.,Vishnyakov A.* Simulation of surfactant adsorption at liquid-liquid interface: what we may expect from soft-core models? // J. Chem. Phys. 2022. №. P. 094706.

[7] *Faria B.F., Palyulin V.V.,Vishnyakov A.M.* Free energies of polymer brushes with mobile anchors in a good solvent calculated with the expanded ensemble method // Colloids and Surfaces A: Physicochemical and Engineering Aspects. 2022. V. 649 №. P. 129443.

[8] *Vishnyakov A., Mao R.F., Kam K., Potanin A., Neimark A.V.* Interactions of Crosslinked Polyacrylic Acid Polyelectrolyte Gels with Nonionic and Ionic Surfactants // Journal of Physical Chemistry B. 2021. V. 125 № 50. P. 13817-13828.

[9] *Vishnyakov A., Weathers T., Hosangadi A.,Chiew Y.C.* Molecular models for phase equilibria of alkanes with air components and combustion products I. Alkane mixtures with nitrogen, CO2 and water // Fluid Phase Equilibria. 2020. V. 514 №. P. 112553.

[10] *Vishnyakov A., Weathers T., Hosangadi A.,Chiew Y.* Molecular models for phase equilibria of alkanes with air components and combustion products II. Alkane–Oxygen mixtures // Fluid Phase Equilibria. 2020. V. 520 №. P. 112650.
[11] *Santo K.P.,Vishnyakov A.* Reversible aggregation of particles with short oligomeric sidechains at the surface studied with Langevin dynamics // Colloids and Surfaces a-Physicochemical and Engineering Aspects. 2020. V. 586 №. P. 124143.
[12] Landers J., Neimark A.V., Asefa T., Vishnyakov A., Goswami A.,Ortiz J.C., *Multicatalyst Polyelectrolyte Membranes and Materials and Methods Utilizing the Same*. 2020, Rutgers University: US.
[13] *Burgess S., Wang Z.J., Vishnyakov A.,Neimark A.V.* Adhesion, intake, and release of nanoparticles by lipid bilayers // Journal of Colloid and Interface Science. 2020. V. 561 №. P. 58-70.
[14] Weathers T., Vishnyakov A., Chiew Y.,Hosangadi A., *Characterizing Thermodynamic Properties of Pure Components and Binary Mixtures at Rocket Conditions Using Molecular Dynamics*, in *Proceedings of AIAA Scitech 2019 Forum*. 2019. p. 1284.
[15] *Santo K.P., Vishnyakov A., Brun Y.,Neimark A.V.* Critical Conditions of Adhesion and Separation of Functionalized Nanoparticles on Polymer Grafted Substrates // Journal of Physical Chemistry C. 2019. V. 123 № 26. P. 16091-16106.
[16] *Vishnyakov A., Mao R., Lee M.T.,Neimark A.V.* Coarse-grained model of nanoscale segregation, water diffusion, and proton transport in Nafion membranes // Journal of Chemical Physics. 2018. V. 148 № 2. P. 024108.
[17] *Santo K.P., Vishnyakov A., Kumar R.,Neimark A.V.* Elucidating the Effects of Metal Complexation on Morphological and Rheological Properties of Polymer Solutions by a Dissipative Particle Dynamics Model // Macromolecules. 2018. V. 51 № 14. P. 4987-5000.
[18] *Santo K.P., Vishnyakov A., Brun Y.,Neimark A.V.* Adhesion and Separation of Nanoparticles on Polymer-Grafted Porous Substrates // Langmuir. 2018. V. 34 № 4. P. 1481-1496.
[19] *Burgess S., Vishnyakov A., Tsovko C.,Neimark A.V.* Nanoparticle-Engendered Rupture of Lipid Membranes // Journal of Physical Chemistry Letters. 2018. V. 9 № 17. P. 4872-4877.
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[21] *Raman A.S., Vishnyakov A.,Chiew Y.C.* A coarse-grained model for PCL: conformation, self-assembly of MePEG-b-PCL amphiphilic diblock copolymers // Molecular Simulation. 2017. V. 43 № 2. P. 92-101.
[22] *Lee M.-T., Vishnyakov A.,Neimark A.V.* Coarse-grained model of water diffusion and proton conductivity in hydrated polyelectrolyte membrane // Journal of Chemical Physics. 2016. V. 144 № 1. P. 014902.
[23] *Lee M.T., Mao R.F., Vishnyakov A.,Neimark A.V.* Parametrization of Chain Molecules in Dissipative Particle Dynamics // Journal of Physical Chemistry B. 2016. V. 120 № 22. P. 4980-4991.
[24] *Landers J., Colon-Ortiz J., Zong K., Goswami A., Asefa T., Vishnyakov A.,Neimark A.V.* In Situ Growth and Characterization of Metal Oxide Nanoparticles within Polyelectrolyte Membranes // Angewandte Chemie-International Edition. 2016. V. 55 № 38. P. 11522-11527.

[25] *Mao R., Lee M.-T., Vishnyakov A.,Neimark A.V.* Modeling Aggregation of Ionic Surfactants Using a Smeared Charge Approximation in Dissipative Particle Dynamics Simulations // Journal of Physical Chemistry B. 2015. V. 119 № 35. P. 11673-11683.
[26] *Lee M.-T., Vishnyakov A.,Neimark A.V.* Modeling Proton Dissociation and Transfer Using Dissipative Particle Dynamics Simulation // Journal of Chemical Theory and Computation. 2015. V. 11 № 9. P. 4395-4403.
[27] *Gor G.Y., Cannarella J., Leng C.Z., Vishnyakov A.,Arnold C.B.* Swelling and softening of lithium-ion battery separators in electrolyte solvents // Journal of Power Sources. 2015. V. 294 №. P. 167-172.
[28] *Cheng J.L., Vishnyakov A.,Neimark A.V.* Adhesion of nanoparticles to polymer brushes studied with the ghost tweezers method // Journal of Chemical Physics. 2015. V. 142 № 3. P. 034705.
[29] *Vishnyakov A.,Neimark A.V.* Self-Assembly in Nafion Membranes upon Hydration: Water Mobility and Adsorption Isotherms // Journal of Physical Chemistry B. 2014. V. 118 № 38. P. 11353-11364.
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[39] *Yang S.A., Vishnyakov A.,Neimark A.V.* Self-assembly in block polyelectrolytes // Journal of Chemical Physics. 2011. V. 134 № 5.
[40] *Vishnyakov A., Gor G.Y., Lee M.T.,Neimark A.V.* Molecular Modeling of Organophosphorous Agents and Their Aqueous Solutions // Journal of Physical Chemistry A. 2011. V. 115 № 20. P. 5201-5209.

[41] *Rasmussen C.J., Vishnyakov A.,Neimark A.V.* Monte Carlo simulation of polymer adsorption // Adsorption-Journal of the International Adsorption Society. 2011. V. 17 № 1. P. 265-271.
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[47] *Vishnyakov A.,Neimark A.V.* Specifics of solvation of sulfonated polyelectrolytes in water, dimethylmethylphosphonate, and their mixture: A molecular simulation study // Journal of Chemical Physics. 2008. V. 128 № 16. P. 164902.
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[50] *Neimark A.V.,Vishnyakov A.* Phase transitions and criticality in small systems: Vapor-liquid transition in nanoscale spherical cavities // Journal of Physical Chemistry B. 2006. V. 110 № 19. P. 9403-9412.
[51] *Ravikovitch P.I., Vishnyakov A., Neimark A.V., Carrott M.R., Russo P.A.,Carrott P.J.* Calculation of pore size distributions in low-k films. in *AIP Conference Proceedings: 5th Conference on Characterization and Metrology for ULSI Technology*. 2005. Richardson, TX: Amer Inst Physics.
[52] *Neimark A.V.,Vishnyakov A.* A simulation method for the calculation of chemical potentials in small, inhomogeneous, and dense systems // Journal of Chemical Physics. 2005. V. 122 № 23. P. 234108.
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Research financial support history

указаны только проекты с ведущей ролью руководителя, со-руководителя, ведущего исполнителя

Support:	Current	Pending	Submission Planned in Near Future	Transfer of Support

Project/Proposal Title:

НЦМУ: Рациональное освоение запасов жидких углеводородов планет (Center of excellence: Rational development of the planet's liquid hydrocarbon reserves)

Source of Support: Минобрнауки (Ministry of Science and Higher Education of Russian Federation) 075-10-2022-011

Total Award Amount: RR 2 mil Total Award Period Covered: 01.01.22-12.31.22

Location of Project: Skoltech Role: Direction leader

Person-Months Per Year Committed to the Project. Cal 2 Acad: NA Sumr: NA

Support:	Current	Pending	Submission Planned in Near Future	Transfer of Support

Project/Proposal Title:

Исследование влияния ионной жидкости в составе электролита на механизм и кинетику реакции восстановления кислорода: на пути к улучшению Li-O2 аккумуляторов (Investigation of the effect of ionic liquid in the electrolyte composition on the mechanism and kinetics of the oxygen reduction reaction: on the way to improving Li-O2 batteries)

Source of Support: РФФИ (Russian Fund for Fundamental Research) 1-RFBR-3441 (PhD student support grant)

Total Award Amount: RR 2 mil Total Award Period Covered: 01.01.20-12.31.22

Location of Project: Skoltech Role PI

Person-Months Per Year Committed to the Project. Cal 1 Acad: NA Sumr: NA

Support:	Current	Pending	Submission Planned in Near Future	Transfer of Support

Project/Proposal Title:

Разработка и апробация подходов к ускорению мультифизических расчетов на примере моделирования кинетики горения водородосодержащей смеси с использованием алгоритмов аппроксимации решения, основанных на базе новых принципов интеллектуального математического моделирования (“Development and approbation of approaches to acceleration of multiphysical calculations by the example of modeling the kinetics of combustion of a hydrogen-containing mixture using algorithms for approximation of the solution, based on new principles of intellectual mathematical modeling”)

Source of Support: Росатом (Rosatom) award FA9550-15-C-0028

Total Award Amount: RR 4.3 mil Total Award Period Covered: 06.01.22-12.31.22

Location of Project: Skoltech Role PI

Person-Months Per Year Committed to the Project. Cal 1 Acad: NA Sumr: NA

Support:	Current	Pending	Submission Planned in Near Future	Transfer of Support

Project/Proposal Title:

Многоклассовая сегментация при построении трехмерных моделей горных пород

Source of Support: Digital core initiative (subproject)

Total Award Amount: R 2 mil Total Award Period Covered: 01.01.22-03.31.22

Location of Project: Skoltech

Person-Months Per Year Committed to the Project. Cal 1 Acad: NA Sumr: NA

Support:	Current	Pending	Submission Planned in Near Future	Transfer of Support

Project/Proposal Title:

Моделирование смачиваемости на границе минерал-нефть-вода в экстремальных условиях (wetting on mineral – brine – crude oil interfaces at reservoir conditions”)

Source of Support: Digital core initiative (subproject)

Total Award Amount: R 6 mil Total Award Period Covered: 01.01.20-03.31.21

Location of Project: Skoltech Role Subproject leader

Person-Months Per Year Committed to the Project. Cal 2 Acad: NA Sumr: NA

Support:	Current	Pending	Submission Planned in Near Future	Transfer of Support

Project/Proposal Title:

Разработка рекомендаций по технологиям извлечения ванадия и никеля из металлургического шлака и нефтяного

сырья (Recommendations on V & Ni extraction from crude oil demetallation wastes)
Source of Support: АО Северсталь (Severstal)
Total Award Amount: R 2.4 mil Total Award Period Covered: 01.01.20-03.31.20
Location of Project: Skoltech Role PI
Person-Months Per Year Committed to the Project. Cal NA Acad: 2 Sumr: NA

Support: Current Pending Submission Planned in Near Future Transfer of Support

Project/Proposal Title:
Phase Transitions, Nucleations and Mixing Modeling through Trans-Critical Conditions
Source of Support: AFOSR (STTR-II FA9550-15-C-0028)
Total Award Amount: $2,009,881 Total Award Period Covered: 01.01.17-12.31.20
Location of Project: Rutgers Role: Faculty
Person-Months Per Year Committed to the Project. Cal NA Acad: 6 Sumr: NA

Project/Proposal Title:
Building theoretical foundations of nanoparticle chromatography with mesoscale simulations
Source of Support: NSF (computer resources time only)
Total Award Amount: $13800 ($ equivalent) Total Award Period Covered: 01.01.17-12.31.17
Location of Project: Rutgers Role: Faculty/SP
Person-Months Per Year Committed to the Project. NA

Project/Proposal Title: GOALI: Theoretical Foundations of Interaction Nanoparticle Chromatography
Source of Support: NSF CBET 1510993
Total Award Amount: $ 300,000 Total Award Period Covered: 09.01.2015 -08.31.2018
Location of Project: Rutgers Role: Faculty/SP
Person-Months Per Year Committed Cal: Acad: Sumr: 1

Support: Current Pending Submission Planned in Near Future Transfer of Support

Project/Proposal Title: Mechanisms of asphaltene precipitation from oil: a multiscale simulation study
Source of Support: ACS PRF
Total Award Amount: $ 110,000 Total Award Period Covered: 09.01.2014 -08.31.2016
Location of Project: Rutgers Role: PI
Person-Months Per Year Committed Cal: Acad: Sumr: 1

Support: Current Pending Submission Planned in Near Future Transfer of Support

Project/Proposal Title: Mass Transport, Kinetics, and Catalytic Activities of Multicatalyst Polyelectrolyte Membranes
Source of Support: DTRA (HDTRA1-14-1-0015)
Total Award Amount: $ 2,209,903 Total Award Period Covered: 02.06.2014-2.5.2018
Location of Project: Rutgers Role: Faculty/SP
Person-Months Per Year Committed Cal: Acad: 3 Sumr:

Support: Current Pending Submission Planned in Near Future Transfer of Support

Project/Proposal Title: Adhesion and Translocation of Nanoparticles through Lipid Membranes
Source of Support: NSF – CBET 1264702
Total Award Amount: $ 349,976 Total Award Period Covered: 08.15.2013-08.30.2016
Location of Project: Rutgers Role: Faculty/SP
Person-Months Per Year Committed Cal: Acad: 0 Sumr: 1

Support: Current Pending Submission Planned in Near Future Transfer of Support

Project/Proposal Title: Mesoscale modeling of self-assembly and transport in polymer electrolyte membranes
Source of Support: NSF – DMR 1207239
Total Award Amount: $383,803 Total Award Period Covered: 09.01.2012-08.31.2015
Location of Project: Rutgers Role: Faculty/SP

Person-Months Per Year Committed				Cal:	Acad: 1 Sumr:
Support:	Current	Pending	Submission Planned in Near Future		Transfer of Support
Project/Proposal Title: Multiscale Modeling of Adsorption Equilibrium and Dynamics in Polymer Chromatography					
Source of Support: NSF					
Total Award Amount: $ 300,000			Total Award Period Covered: 7.1.2011-6.30.2014		
Location of Project: Rutgers		Role: Faculty/SP			
Person-Months Per Year Committed to the Project.			2	Cal:	Acad: Sumr: 1
Support:	Current	Pending	Submission Planned in Near Future		Transfer of Support
Project/Proposal Title: Computer Laboratory for Modeling of Nanostructured Polymeric Materials (DURIP)					
Source of Support: ARO (capital equipment only)					
Total Award Amount: $100000			Total Award Period Covered: 09.01.2012-08.31.2013		
Location of Project: Rutgers		Role: Faculty/SP			
Person-Months Per Year Committed to the Project.			0	Cal: 0	Acad: Sumr: 0
Support:	Current	Pending	Submission Planned in Near Future		Transfer of Support
Project/Proposal Title: Multiscale Modeling of Permeability of Protective Polyelectrolyte Membranes to CBW agents					
Source of Support: DTRA					
Total Award Amount: $750000			Total Award Period Covered: 07.01.08-06.30.11		
Location of Project: Rutgers		Role: Faculty/SP			
Person-Months Per Year Committed to the Project.			4.5	Cal: 3.5	Acad: Sumr: 1

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Вишняков А.М.

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16 августа 2022 г