Nikolai Volkov

Department of Statistical Physics
Faculty of Physics
Saint Petersburg State University
198504 Saint Petersburg, Russia

☎ +7 812 428 4515 (office)
✉ nikolay.volkov@spbu.ru

Research interests

Statistical physics, thermodynamics, molecular dynamics and Monte Carlo methods, surfactants, micelles, chemical potential, diffusion, viscosity, interfacial tension

Employment

Sep.2017–present	Associate Professor. Department of Statistical Physics, Faculty of Physics, Saint Petersburg State University, Russia.
Aug.2015–Sep.2017	Senior Research Fellow. Department of Statistical Physics, Faculty of Physics, Saint Petersburg State University, Russia.
Aug.2013–Aug.2015	Postdoctoral researcher. Department of Statistical Physics, Faculty of Physics, Saint Petersburg State University.
Jan.2011–Jan.2013	Postdoctoral researcher. Division of Physical Chemistry, Department of Chemistry and Molecular Biology, University of Gothenburg, Sweden.
Oct.2008–Dec.2010	Postdoctoral researcher. Division of Physical Chemistry, Department of Materials and Environmental Chemistry, Stockholm University, Sweden.
Apr.2007–Sep.2008	Programmer. PROMT, Automated Translation Solutions, Saint Petersburg, Russia.
Jan.2006–Apr.2007	Research assistant. Department of Statistical Physics, Faculty of Physics, Saint Petersburg State University.
Jan.2003–Dec.2005	PhD student. Department of Statistical Physics, Faculty of Physics, Saint Petersburg State University.

Education

Department of Statistical Physics, Faculty of Physics, Saint Petersburg State University

October 25, 2007	PhD degree in Physics.
November 20, 2002	Master of Science degree in Physics (with honours).
June 14, 2000	Bachelor of Science degree in Physics (with honours).

Teaching

- Delivers lectures on "Non-equilibrium thermodynamics and the projecting operators method" for the 4th year undergraduate students at the Department of Statistical Physics, Saint Petersburg State University.
- Leads seminars on "Statistical Physics and Thermodynamics" for the 3rd and 4th year undergraduate students at the Faculty of Physics, Saint Petersburg State University.

Grants

- Russian Science Foundation, grant 22-13-00151 "On the microscopic theory of the formation of thermodynamically stable bubbles and droplets near a solid surface", co-investigator, 05.2022–12.2024.
- Russian Foundation for Basic Research, competition "A" (Projects for basic scientific research), 20-03-00641 A "Development of thermodynamics and kinetics of micellization in non-polar media", co-investigator, 03.2020–12.2022.
- Russian Foundation for Basic Research, competition "YaF_a" (Competition of joint initiative Russian-Japanese scientific projects), 18-53-50015 YaF_a "The mechanism of molecular adsorption of water on the small spherical particles: the effects of wetting, size and roughness, electrical contributions from adsorbed charges and dipoles", co-investigator, 02.2018–04.2020.
- Russian Science Foundation, "Thermodynamic, kinetic and molecular modeling of micelles and processes in micellar systems", grant 14-13-00112, co-investigator, 2014–2018.
- Russian Foundation for Basic Research, "Experimental and theoretical study of diffusion kinetics in micellar solutions", grant 13-03-00991, co-investigator, 2013–2015.
- Saint Petersburg State University's conference grant for participation in the 28-th European Symposium on Applied Thermodynamics (Athens, Greece, 2015).
- Saint Petersburg State University's conference grant for participation in the 20th International Symposium on Surfactants in Solution (Coimbra, Portugal, 2014).
- Russian Foundation for Basic Research, "Computer simulation of molecular nanosystems in the framework of classical and quantum statistics", grant 08-02-00041, co-investigator, 2008–2010.
- Russian Foundation for Basic Research, "Simulation of molecular systems by generalized ensembles Monte Carlo methods", grant 05-02-17428, co-investigator, 2005–2007.
- Competitive Center for Fundamental Science at St.Petersburg State University, "Monte Carlo simulation of polymer systems in generalized ensembles", PhD student's personal grant, 2004.
- Russian Foundation for Basic Research, "Computer simulation of molecular systems in the framework of classical and quantum statistics", grant 02-02-16618, co-investigator, 2002–2004.

Scientific visits

Apr.2019	Department of Chemistry, Okayama University, Japan
Dec.2018	Freie Universität Berlin, Germany
Apr.2018	Department of Mechanical Engineering, Keio University, Japan
Jun.2017	Soft Matter & Molecular Biophysics Group, Department of Applied Physics, Faculty of Physics, University of Santiago de Compostela, Spain.
Oct.2016	Department of Mechanical Engineering, Keio University, Japan
Sep.2015–Oct.2015	Soft Matter & Molecular Biophysics Group, Department of Applied Physics, Faculty of Physics, University of Santiago de Compostela, Spain.
Apr.2015	Division of Physical Chemistry, Department of Materials and Environmental Chemistry, Stockholm University, Sweden.
Apr.2005–Sep.2005	Division of Physical Chemistry, Department of Materials and Environmental Chemistry, Stockholm University, Sweden.

Publications

Papers

Number of papers: 22, h-index (Scopus): 10.
https://www.scopus.com/authid/detail.uri?authorId=9248780800
http://www.researcherid.com/rid/B-5863-2012
https://scholar.google.ru/citations?user=Aks1NqAAAAAJ&hl=en
http://orcid.org/0000-0001-7419-8783

1. A.A. Vanin, N.A. Volkov, E.N. Brodskaya, A.K. Shchekin, E.A. Turnaeva, M.S. Polovinkin, and Yu.A. Eroshkin. Molecular Dynamics Calculation of Interfacial Tension in a Two-Phase Liquid Hydrocarbon–Water–Surfactant System: From Rarefied to Superdense Surfactant Monolayer. Russian Journal of Physical Chemistry A, 2024, Vol. 98, No. 9, pp. 1997–2006. DOI: 10.1134/S0036024424701139

2. M.S. Polovinkin, N.A. Volkov, D.V. Tatyanenko, A.K. Shchekin. Contact angle calculations for argon and water sessile droplets on planar lyophilic and lyophobic surfaces within molecular dynamics modeling. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2024, Vol. 702, 134932. https://doi.org/10.1016/j.colsurfa.2024.134932

3. A.G. Bykov, M.A. Panaeva, A.R. Rafikova, N.A. Volkov, and A.A. Vanin. Influence of Composition and Temperature on Dynamic Properties of Mixed Monolayers of Pulmonary Lipids. Colloid Journal, 2024, Vol. 86, No. 1, pp. 14–22. https://doi.org/10.1134/S1061933X23601142

4. A.K. Shchekin, L.Ts. Adzhemyan, Yu.A. Eroshkin, N.A. Volkov. Work of Formation of Direct and Inverse Micelle as a Functions of Aggregation Number. Colloid Journal, 2022, Vol. 84, No. 1, pp. 109-119. DOI: 10.1134/S1061933X22010124

5. N.A. Volkov, Yu.A. Eroshkin, A.K. Shchekin, I.N. Koltsov, N.Yu. Tretyakov, E.A. Turnaeva, S.S. Volkova, and A.A. Groman. Molecular Dynamics of Decane Solubilization and Diffusion of Aggregates Consisting of Surfactant and Decane Molecules in Aqueous Solutions. Colloid Journal, 2021, Vol. 83, No. 4, pp. 406-417. DOI: 10.1134/S1061933X21040141

6. A.K. Shchekin, N.A. Volkov, I.N. Koltsov, N.Yu. Tretyakov, S.S. Volkova, and E.A. Turnaeva. Molecular-Thermodynamic Model of Solubilization in Direct Spherical Micelles of Nonionic Surfactants. Colloid Journal, 2021, Vol. 83, No. 4, pp. 518-529. DOI: 10.1134/S1061933X21040128

7. Volkov, N.A., Gonorovskaya, E.V., Shchekin, A.K., Vorontsov-Velyaminov, P.N. Calculation of Chemical Potential of a Molecule on the Basis of Radial Distribution Functions, Colloid Journal, 2020, 82(6), pp. 634-640, DOI: 10.1134/S1061933X20060198

8. Shchekin, A.K., Koga, K., Volkov, N.A. The effect of a finite number of monomers available for aggregation at nucleation and micellization in a fixed volume, Journal of Chemical Physics, 2019, 151(24), 244903, DOI: 10.1063/1.5129160

9. Volkov, N.A., Posysoev, M.V., Shchekin, A.K. The Effect of Simulation Cell Size on the Diffusion Coefficient of an Ionic Surfactant Aggregate, Colloid Journal, 2018, 80(3), pp. 248-254, DOI: 10.1134/S1061933X1803016X

10. Shchekin, A.K., Adzhemyan, L.T., Babintsev, I.A., Volkov, N.A. Kinetics of Aggregation and Relaxation in Micellar Surfactant Solutions, Colloid Journal, 2018, 80(2), pp. 107-140, DOI: 10.1134/S1061933X18020084

11. Rusanov, A.I., Shchekin, A.K., Volkov, N.A. Diffusion in micellar systems: Theory and molecular modelling, Russian Chemical Reviews, 2017, 86(7), pp. 567-588, DOI: 10.1070/RCR4736

12. N.Volkov, A.Shchekin, N.Tuzov, T.Lebedeva, M.Kazantseva "Molecular modeling of ionic aggregates at several concentrations of SDS in aqueous solution", Journal of Molecular Liquids, 2017, Vol. 236, pp. 414–421. DOI: 10.1016/j.molliq.2017.04.018.

13. N.A.Volkov, N.V.Tuzov, A.K.Shchekin "All-Atom Molecular Dynamics Analysis of Kinetic and Structural Properties of Ionic Micellar Solutions", Colloid Journal, **79**, No. 2, 181–189 (2017).

14. N.A.Volkov, N.V.Tuzov, A.K.Shchekin "Molecular dynamics study of salt influence on transport and structural properties of SDS micellar solutions", Fluid Phase Equilib., **424**, 114–121 (2016).

15. Nikolai A. Volkov, Boris B. Divinskiy, Pavel N. Vorontsov-Velyaminov, Alexander K. Shchekin, "Diffusivities of species in ionic micellar solutions: molecular dynamic simulation", Colloids and Surfaces A: Physicochem. Eng. Aspects, **480**, 165–170 (2015).

16. A.K. Shchekin, I.A. Babintsev, L.Ts. Adzhemyan, N.A. Volkov, "Kinetic modeling of self-aggregation in solutions with coexisting spherical and cylindrical micelles at arbitrary initial conditions", RSC Advances, **4**, 51722–51733 (2014).

17. N. Volkov, A. Lyubartsev and L. Bergström "Phase transitions and thermodynamic properties of dense assemblies of truncated nanocubes and cuboctahedra", Nanoscale, **4**, 4765–4771 (2012).

18. N.A. Volkov, P.N. Vorontsov-Velyaminov and A.P. Lyubartsev "Two-Dimensional Wang-Landau Algorithm for Osmotic Pressure Calculations in a Polyelectrolyte-Membrane System", Macromolecular Theory and Simulations, **20**, 496–509 (2011).

19. P.N. Vorontsov-Velyaminov, N.A. Volkov, A.A. Yurchenko, A.P. Lyubartsev, "Simulation of polymers by the Monte Carlo method using the Wang-Landau algorithm", Polymer Science, Ser. A, **52**, No.7, 742–760 (2010).

20. N.A. Volkov, P.N. Vorontsov-Velyaminov, A.P. Lyubartsev "Entropic sampling of flexible polyelectrolytes within the Wang-Landau algorithm", Physical Review E, **75**, 016705 (2007);
DOI: 10.1103/PhysRevE.75.016705.

21. N.A. Volkov, A.A. Yurchenko, A.P. Lyubartsev, P.N. Vorontsov-Velyaminov "Entropic sampling of free and ring polymer chains". Macromolecular Theory and Simulations, **14**, 491–504 (2005).

22. P.N. Vorontsov-Velyaminov, N.A. Volkov, A.A. Yurchenko "Entropic sampling of simple polymer models within Wang-Landau algorithm". Journal of Physics A: Mathematical and General, **37**, 1573–1588 (2004).

Book chapters

- P.N. Vorontsov-Velyaminov, N.A. Volkov, A.A. Yurchenko, A.P. Lyubartsev, "Monte Carlo simulations of polymers in generalized ensembles" in "Application of computer simulation methods for the study of polymers and biopolymers", Eds. V.A. Ivanov, A.L. Rabinovich, A.R. Khokhlov, KD Librocom (2009), in Russian.

PhD thesis

- N.A. Volkov "A study of equilibrium properties within lattice models of an uncharged polymer and of a polyelectrolyte by Monte Carlo method with the aid of Wang-Landau algorithm", Saint Petersburg State University (2007).

Computer skills

Programming	Perl, C++
IDE	NetBeans
Simulations	GROMACS, MDynaMix
Graphics	Gnuplot, Inkscape
Publishing	LaTeX
Operating systems	Linux