

N.A. Volkov. Publications

Papers

<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. Tatyanyenko, 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).