

РЕЛАКСАЦИЯ СОЛЬВАТНЫХ ОБОЛОЧЕК ИОНОВ В СМЕСИ ЖИДКОСТЕЙ

- [1] The effect of a mixture of an ionic liquid and organic solvent on oxygen reduction reaction kinetics / Pavlov Sergey, Danilova Valentina, Sivakov Vyacheslav, and Kislenko Sergey // *Phys. Chem. Chem. Phys.* — 2022. — Vol. 24, no. 27. — P. 16746–16754. — Access mode: <http://dx.doi.org/10.1039/D2CP00698G>.
- [2] Zhiyi Gao, Zongjing Lu, Yining Zhang, Jing Xia, Xuejing Zhang, Chao Sun, Yijun Yang, Yong Xu, Ke Wang, Xi Wang Jiannian Yao. Regulating interfacial desolvation via a weakly coordinating solvent molecule enhances Li-ion storage at subzero temperatures // *Chem. Eng. Sci.* — 2022. — Vol. 254. — P. 117633.
- [3] Orekhov M A. Effect of divalent ion coordination on ion diffusion in organic liquids // *J. Mol. Liq.* — 2021. — Vol. 343. — P. 117647. — Access mode: <https://doi.org/10.1016/j.molliq.2021.117647>.
- [4] Orekhov M A. Fluctuation enhancement of ion diffusivity in liquids // *Phys. Chem. Chem. Phys.* — 2017. — Vol. 19. — P. 32398–32403. — Access mode: <http://dx.doi.org/10.1039/C7CP07170A>.
- [5] Liu Hongjun, Maginn Edward. Effect of ion structure on conductivity in lithium-doped ionic liquid electrolytes: A molecular dynamics study // *J. Chem. Phys.* — 2013. — Vol. 139, no. 11. — P. 114508.
- [6] Prediction of dynamics properties of ThF₄-based fluoride molten salts by molecular dynamic simulation / Dai Jian-xing, Zhang Wei, Ren Cui-lan, and Guo Xiao-jing // *J. Mol. Liq.* — 2020. — P. 114059. — Access mode: <https://doi.org/10.1016/j.molliq.2020.114059>.
- [7] Smirnov Vladimir, Kislenko Sergey. Effect of Cation Size on Solvation and Association with Superoxide Anion in Aprotic Solvents // *ChemPhysChem.* — 2019. — Vol. 20. — P. 1960–1966. — Access mode: <https://onlinelibrary.wiley.com/doi/abs/10.1002/cphc.201900389>.
- [8] Kumar Parveen, Yashonath S. Ionic conductivity in aqueous electrolyte solutions: Insights from computer simulations // *J. Mol. Liq.* — 2019. — Vol. 277. — P. 506–515. — Access mode: <https://doi.org/10.1016/j.molliq.2018.12.090>.
- [9] Towards high throughput screening of electrochemical stability of battery electrolytes / Borodin Oleg, Olguin Marco, Spear Carrie E., Leiter Kenneth W., and Knap Jaroslaw // *Nanotechnology.* — 2015. — Vol. 26, no. 35. — P. 354003. — Access mode: <http://dx.doi.org/10.1088/0957-4484/26/35/354003>.
- [10] Structure, dynamics and ionic conductivities of ternary ionic liquid/lithium salt/DMSO mixtures / Martínez-Crespo Pablo, Otero-Lema Martín, Cabeza Oscar, Montes-Campos Hadrián, and Varela Luis M. // *J. Mol. Liq.* — 2022. — Vol. 359. — P. 119188.
- [11] Molecular dynamics simulation of ion binding in aqueous solution of 18-crown-6 ether / Bakulin I. K., Kondratyuk N. D., Lankin A. V., and Norman G. E. // *J. Phys.: Conf. Ser.* — 2021. — Vol. 1787, no. 1.
- [12] Kondratyuk N D, Norman G E, Stegailov V V. Microscopic Mechanisms of Diffusion of Higher Alkanes // *Polymer Science Series A.* — 2016. — Vol. 56, no. 5. — P. 825–836.
- [13] Kondratyuk Nikolay D., Norman Genri E., Stegailov Vladimir V. Self-consistent molecular dynamics calculation of diffusion in higher n -alkanes // *J. Chem. Phys.* — 2016. — Vol. 145, no. 20. — P. 204504. — Access mode: <http://dx.doi.org/10.1063/1.4967873>.
- [14] Garkul Anastasiia, Stegailov Vladimir. Molecular dynamics analysis of elastic properties and new phase formation during amorphous ices transformations // *Sci. Rep.* — 2022. — Vol. 12. — P. 13325. — Access mode: <https://doi.org/10.1038/s41598-022-17666-2>.
- [15] Standards for molecular dynamics modelling and simulation of relaxation / Kuksin A. Y., Morozov I. V., Norman G. E., Stegailov V. V., and Valuev I. A. // *Mol Simul.* — 2005. — Vol. 31, no. 14-15. — P. 1005–1017.
- [16] Lankin A V, Norman G E, Orekhov M A. Temporal and spatial properties of ion solvation in simple liquids // *Journal of Physics: Conference Series.* — 2015. — Vol. 653. — P. 12155. — Access mode: <http://stacks.iop.org/1742-6596/653/i=1/a=012155?key=crossref.305aca7afb24a721902f0c5f935e109>.
- [17] Орехов М. А. Координационные Числа Двухвалентных Ионов В Органических Растворителях // *ЖФХ.* — 2021. — Т. 95, № 10. — С. 1538–1543.
- [18] Reddy Sandeep K., Balasubramanian Sundaram. Liquid dimethyl carbonate: A quantum chemical and molecular dynamics study // *J. Phys. Chem. B.* — 2012. — Vol. 116, no. 51. — P. 14892–14902.
- [19] Klasczyk Benjamin, Knecht Volker. Kirkwood-Buff derived force field for alkali chlorides in simple point charge water // *J. Chem. Phys.* — 2010. — Vol. 132, no. 2. — P. 0–12.
- [20] Kuzmina E. V., Karaseva E. V., Kolosnitsyn V. S. Molecular Dynamics Studies of the Physicochemical Properties and Structure of the 1 M LiClO₄ Solution in Sulfolane // *Russ. J. Phys. Chem. A.* — 2022. — Vol. 96, no. 1. — P. 115–124.
- [21] Berendsen H.J.C., van der Spoel D, van Drunen R. GROMACS: A message-passing parallel molecular dynamics implementation // *Comput. Phys. Commun.* — 1995. — Vol. 91, no. 1-3. — P. 43–56.
- [22] Jorgensen William L., Maxwell David S., Tirado-Rives Julian. Development and testing of the OPLS all-atom force field on conformational energetics and properties of organic liquids // *J. Am. Chem. Soc.* — 1996. — Vol. 118, no. 45. — P. 11225–11236.
- [23] An Automated Force Field Topology Builder (ATB) and Repository: Version 1.0 / Malde Alpeshkumar K, Zuo Le, Breeze Matthew, Stroet Martin, Poger David, Nair Pramod C, Oostenbrink Chris, and Mark Alan E // *J. Chem. Theory Comput.* — 2011. — Vol. 7, no. 12. — P. 4026–4037.
- [24] LigParGen web server: an automatic OPLS-AA parameter generator for organic ligands / Doddla Leela S., Cabeza de Vaca Israel, Tirado-Rives Julian, and Jorgensen William L. // *Nucleic Acids Research.* — 2017. — 04. —

Vol. 45, no. W1.—P. W331–W336.—Access mode: <https://doi.org/10.1093/nar/gkx312>.

- [25] Yeh In-Chul, and Gerhard Hummer. System-Size Dependence of Diffusion Coefficients and Viscosities from Molecular Dynamics Simulations with Periodic Boundary Conditions // J. Phys. Chem. B.—2004.—Vol. 108, no. 40.—P. 15873.—Access mode: <http://dx.doi.org/10.1021/jp0477147>.
- [26] Yeh In-Chul, Hummer Gerhard. Diffusion and electrophoretic mobility of single-stranded RNA from molecular dynamics simulations. // Biophys. J.—2004.—Vol. 86, no. 2.—P. 681–689.—Access mode: [http://dx.doi.org/10.1016/S0006-3495\(04\)74147-8](http://dx.doi.org/10.1016/S0006-3495(04)74147-8).
- [27] Dünweg Burkhard, Kremer Kurt. Molecular dynamics simulation of a polymer chain in solution // J. Chem. Phys.—1993.—Vol. 99, no. 9.—P. 6983–6997.
- [28] Orekhov M. A. Improving molecular dynamics calculation of diffusivity in liquids with theoretical models // J. Mol. Liq.—2021.—Vol. 322.—P. 114554.
- [29] Smirnov Vladimir S., Kislenko Sergey A. Effect of Solvents on the Behavior of Lithium and Superoxide Ions in Lithium-Oxygen Battery Electrolytes // Chem. Phys. Chem.—2017.—Vol. 19, no. 1.—P. 75–81.—Access mode: <http://doi.wiley.com/10.1002/cphc.201700980>.