

ПЕРСПЕКТИВЫ ВЫЧИСЛИТЕЛЬНОГО СКРИНИНГА УСТОЙЧИВЫХ К РЕАКЦИЯМ НА АНОДЕ РАСТВОРИТЕЛЕЙ ДЛЯ ЛИТИЙ-ИОННЫХ АККУМУЛЯТОРОВ

- [1] Review on modeling of the anode solid electrolyte interphase (SEI) for lithium-ion batteries / Wang Aiping, Kadam Sanket, Li Hong, Shi Siqi, and Qi Yue // *npj Computational Materials*. — 2018. — Vol. 4, no. 1. — P. 15. — Access mode: <http://dx.doi.org/10.1038/s41524-018-0064-0>.
- [2] Yu Zhiao et al. Molecular design for electrolyte solvents enabling energy-dense and long-cycling lithium metal batteries // *Nature Energy*. — 2020. — Vol. 5, no. 7. — P. 526–533. — Access mode: <http://dx.doi.org/10.1038/s41560-020-0634-5>.
- [3] High-Stability Lithium Metal Batteries Enabled by a Tetrahydrofuran-Based Electrolyte Mixture / Paul-Orecchio Austin G., Weeks Jason A., Dolocan Andrei, and Mullins C. Buddie // *ACS Applied Energy Materials*. — 2022. — Vol. 5, no. 8. — P. 9437–9446.
- [4] The physical origin of the activation barrier in Li-ion intercalation processes: the overestimated role of desolvation / Chekushkin Petr M., Merenkov Ivan S., Smirnov Vladimir S., Kislenco Sergey A., and Nikitina Victoria A. // *Electrochimica Acta*. — 2021. — Vol. 372. — P. 137843.
- [5] Solvation sheath reorganization enables divalent metal batteries with fast interfacial charge transfer kinetics / Hou Singyuk, Ji Xiao, Gaskell Karen, Wang Peng Fei, Wang Luning, Xu Jijian, Sun Ruimin, Borodin Oleg, and Wang Chunsheng // *Science*. — 2021. — Vol. 374, no. 6564. — P. 172–178.
- [6] Meng Y. Shirley, Srinivasan Venkat, Xu Kang. Designing better electrolytes // *Science*. — 2022. — Vol. 378, no. 6624.
- [7] Quantum Chemistry-Informed Active Learning to Accelerate the Design and Discovery of Sustainable Energy Storage Materials / Doan Hieu A., Agarwal Garvit, Qian Hai, Counihan Michael J., Rodríguez-López Joaquín, Moore Jeffrey S., and Assary Rajeev S. // *Chemistry of Materials*. — 2020. — Vol. 32, no. 15. — P. 6338–6346.
- [8] Accelerating Electrolyte Discovery for Energy Storage with High-Throughput Screening / Cheng Lei, Assary Rajeev S., Qu Xiaohui, Jain Anubhav, Ong Shyue Ping, Rajput Nav Nidhi, Persson Kristin, and Curtiss Larry A. // *Journal of Physical Chemistry Letters*. — 2015. — Vol. 6, no. 2. — P. 283–291.
- [9] The Electrolyte Genome project: A big data approach in battery materials discovery / Qu Xiaohui, Jain Anubhav, Rajput Nav Nidhi, Cheng Lei, Zhang Yong, Ong Shyue Ping, Brafman Miriam, Maginn Edward, Curtiss Larry A., and Persson Kristin A. // *Computational Materials Science*. — 2015. — Vol. 103. — P. 56–67. — Access mode: <http://dx.doi.org/10.1016/j.commatsci.2015.02.050>.
- [10] Korth Martin. Large-scale virtual high-throughput screening for the identification of new battery electrolyte solvents: Evaluation of electronic structure theory methods // *Physical Chemistry Chemical Physics*. — 2014. — Vol. 16, no. 17. — P. 7919–7926.
- [11] Towards high throughput screening of electrochemical stability of battery electrolytes / Borodin Oleg, Olguin Marco, Spear Carrie E., Leiter Kenneth W., and Knap Jaroslav // *Nanotechnology*. — 2015. — Vol. 26, no. 35. — P. 354003. — Access mode: <http://dx.doi.org/10.1088/0957-4484/26/35/354003>.
- [12] Orekhov M A. Correcting charge distribution in reduced Li-molecule pair for computational screening of battery solvents // *J. Comput. Chem.* — 2023. — P. <https://doi.org/10.1002/jcc.27229>.
- [13] A Thermodynamic Cycle-Based Electrochemical Windows Database of 308 Electrolyte Solvents for Rechargeable Batteries / Wang Da, He Tingting, Wang Aiping, Guo Kai, Avdeev Maxim, Ouyang Chuying, Chen Liquan, and Shi Siqi // *Advanced Functional Materials*. — 2023. — Vol. 33, no. 11. — P. 2212342.
- [14] Agarwal Garvit, Doan Hieu, Assary Rajeev S. Molecular Structure and Electron Affinity of Metal-Solvent Complexes: Insights from Density Functional Theory Simulations // *Journal of The Electrochemical Society*. — 2020. — Vol. 167. — P. 100545.
- [15] Revising the pathways of the Li reaction with organic carbonates / Rulev Alexey A., Frolov Alexander, Doronin Sergey, Bezuglov Iliya, Itkis Daniil M., and Yashina Lada V. // *Physical Chemistry Chemical Physics*. — 2020. — Vol. 22, no. 28. — P. 16184–16192.
- [16] Xu Jijian et al. Electrolyte design for Li-ion batteries under extreme operating conditions // *Nature*. — 2023. — Vol. 614. — P. 694.
- [17] Importance of Reduction and Oxidation Stability of High Voltage Electrolytes and Additives / Delp Samuel A., Borodin Oleg, Olguin Marco, Eisner Claire G., Allen Joshua L., and Jow T. Richard // *Electrochimica Acta*. — 2016. — Vol. 209. — P. 498–510. — Access mode: <http://dx.doi.org/10.1016/j.electacta.2016.05.100>.
- [18] Leung Kevin. Two-electron reduction of ethylene carbonate: A quantum chemistry re-examination of mechanisms // *Chemical Physics Letters*. — 2013. — Vol. 568-569. — P. 1–8. — Access mode: <http://dx.doi.org/10.1016/j.cplett.2012.08.022>.
- [19] PubChem 2023 update / Kim Sunghwan, Chen Jie, Cheng Tiejun, Gindulyte Asta, He Jia, He Siqian, Li Qingliang, Shoemaker Benjamin A., Thiessen Paul A., Yu Bo, Zaslavsky Leonid, Zhang Jian, and Bolton Evan E. // *Nucleic Acids Research*. — 2023. — Vol. 51, no. D1. — P. D1373–D1380.
- [20] Wu Qin, Van Voorhis Troy. Direct optimization method to study constrained systems within density-functional theory // *Physical Review A - Atomic, Molecular, and Optical Physics*. — 2005. — Vol. 72, no. 2. — P. 7–10.
- [21] NWChem: A comprehensive and scalable open-source solution for large scale molecular simulations / Valiev M., Bylaska E. J., Govind N., Kowalski K., Straatsma T. P., Van Dam H. J.J., Wang D., Nieplocha J., Apra E., Windus T. L., and De Jong W. A. // *Computer Physics Communications*. — 2010. — Vol. 181, no. 9. — P. 1477–1489. —

Access mode: <http://dx.doi.org/10.1016/j.cpc.2010.04.018>.

- [22] Zhao Yan, Schultz Nathan E., Truhlar Donald G. Design of Density Functionals by Combining the Method of Constraint Satisfaction with Parametrization for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions // *Journal of Chemical Theory and Computation*. — 2006. — Vol. 2, no. 2. — P. 364–382. — Access mode: <http://pubs.acs.org/doi/abs/10.1021/ct0502763>.
- [23] LigParGen web server: An automatic OPLS-AA parameter generator for organic ligands / Dodda Leela S., De Vaca Israel Cabeza, Tirado-Rives Julian, and Jorgensen William L. // *Nucleic Acids Research*. — 2017. — Vol. 45, no. W1. — P. W331–W336.
- [24] Theoretical studies to understand surface chemistry on carbon anodes for lithium-ion batteries: Reduction mechanisms of ethylene carbonate / Wang Y., Nakamura S., Ue M., and Balbuena P. B. // *Journal of the American Chemical Society*. — 2001. — Vol. 123, no. 47. — P. 11708–11718.
- [25] Atkin Peter, Paula Julio. *Physical chemistry*. — Oxford University Press, 2006. — P. 1072. — ISBN: 978-0716787594.