DAFTAR PUSTAKA

Ando, H., Kojima, T., Takeichi, N., Watanabe, H., Umebayashi, Y., and Senoh, H., 2019, Mixture of monoglyme-based solvent and lithium Bis (trifluoromethanesulfonyl) amide as electrolyte for lithium ion battery using silicon electrode, *Mater. Chem. Phys.*, 225, 105–110.

Armand, M., Axmann, P., Bresser, D., Copley, M., Edström, K., Ekberg, C., Guyomard, D., Lestriez, B., Novák, P., Petranikova, M., Porcher, W., Trabesinger, S., Wohlfahrt-Mehrens, M., and Zhang, H., 2020, Lithium-ion batteries–Current state of the art and anticipated developments, *J. Power Sources*, 479, 228708.

Arshadi, M., Yamdagni, R., and Kebarle, P., 1970, Hydration of the halide negative ions in the gas phase. II. Comparison of hydration energies for the alkali positive and halide negative ions, *J. Phys. Chem.*, 74, 1475.

Aurbach, D., Talyosef, Y., Markovsky, B., Markevich, E., Zinigrad, E., Asraf, L., Gnanaraj, J. S., and Kim, H. J., 2004, Design of electrolyte solutions for Li and Li-ion batteries: a review, *Electrochim. Acta*, 50(2-3), 247-254.

Bae, H., and Kim, Y., 2021, Technologies of lithium recycling from waste lithium ion batteries: a review, *Mater. Adv.*, 2(10), 3234–3250.

Berendsen, H. J., Postma, J. V., Van Gunsteren, W. F., DiNola, A. R. H. J., and Haak, J. R., 1984, Molecular dynamics with coupling to an external bath, *J. Chem. Phys.*, 81(8), 3684–3690.

Best, A. S., Bhatt, A. I., and Hollenkamp, A. F., 2010, Ionic liquids with the bis(fluorosulfonyl)imide anion: electrochemical properties and applications in battery technology, *J. Electrochem. Soc.*, 157(8), A903–A911.

Borodin, O., Suo, L., Gobet, M., Ren, X., Wang, F., Faraone, A., Peng, J., Olguin, M., Schroeder, M., Ding, M. S., Gobrogge E., van Wald Cresce, A., Munoz S., Dura, J A., Greenbaum, S., Wang, C., and Xu, K., 2017, Liquid structure with nano-heterogeneity promotes cationic transport in concentrated electrolytes, *ACS nano*, 11(10), 10462–10471.

Capiglia, C., Saito, Y., Kageyama, H., Mustarelli, P., Iwamoto, T., Tabuchi, T., and Tukamoto, H., 1999, ^{7}Li and ^{19}F diffusion coefficients and thermal properties of non-aqueous electrolyte solutions for rechargeable lithium batteries. *J. Power Sources*, 81, 859–862.

Carrillo-Tripp, M., Saint-Martin, H., and Ortega-Blake, I., 2003, A comparative study of the hydration of Na^+ and K^+ with refined polarizable model potentials, *J. Chem. Phys.*, 118, 7062–7073.

Chen, Y., Wang, J., Flanagan, D. R., 2017, "Fundamental of Diffusion and Dissolution" in *Developing Solid Oral Dosage Forms*, Eds. Qiu, Y., Chen, Y., Zhang, G.G.Z., Yu, L., Mantri, R. V., Academic Press, Cambridge, MA, USA, pp. 253–270.

Chen, M., Feng, G., and Qiao, R., 2020, Water-in-salt electrolytes: An interfacial perspective, *COCIS*, 47, 99–110.

Cresce, A. V., Russell, S. M., Borodin, O., Allen, J. A., Schroeder, M. A., Dai, M., Peng, J., Gobet, M. P., Greenbaum, S. G., Roger, R. E., and Xu, K., 2017, Solvation behavior of carbonate-based electrolytes in sodium ion batteries, *Phys. Chem. Chem. Phys.*, 19(1), 574-586.

Crompton, T.R., 2000, "Introduction to Battery Technology" in *Battery reference book*, Newnes, Oxford, UK, pp. 1–64.

Doherty, B., Zhong, X., Gathiaka, S., Li, B., Acevedo O., 2017, Revisiting OPLS force field parameters for ionic liquid simulations, *J. Chem. Theory Comput.*, 13, 6131–6145.

Dukhin, A., and Pavlenishvilli, D., 2023, "Water-in-salt" super concentrated electrolyte clusters are "micelles", *Colloids Surf., A*, 678, 132466.

Dzidic, I., and Kebarle, P., 1970, Hydration of the alkali ions in the gas phase. Enthalpies and entropies of reactions $M^+(H_2O)_{n-1} + H_2O = M^+(H_2O)_n$, *J. Phys. Chem.*, 74, 1466.

Eilmes, A., and Kubisiak, P., 2015, Stability of ion triplets in ionic liquid/lithium salt solutions: insights from implicit and explicit solvent models and molecular dynamics simulations, *J. Comput. Chem.* 36, 751–762.

Errougui, A., Lahmidi, A., Chtita, S., El Kouali, M., and Talbi, M., 2023, Hydration structures and dynamics of the sodium fluoride aqueous solutions at various temperatures: molecular dynamics simulations, *J. Solution Chem.*, 52(2), 176–186.

Eshetu, G. G., Grugeon, S., Kim, H., Jeong, S., Wu, L., Gachot, G., Laruelle, S., Armand, M., and Passerini, S., 2016, Comprehensive insights into the reactivity of electrolytes based on sodium ions, *ChemSusChem*, 9(5), 462-471.

Fong, K. D., Self, J., McCloskey, B. D., and Persson, K. A., 2020, Onsager transport coefficients and transference numbers in polyelectrolyte solutions and polymerized ionic liquids, *Macromolecules*, 53(21), 9503–9512.

French, M., Hamel, S., and Redmer, R., 2011, Dynamical screening and ionic conductivity in water from *ab initio* simulations,*Phys. Rev. Lett.*, 107, 18591.

France-Lanord, A., and Grossman, J. C., 2019, Correlations from ion pairing and the Nernst-Einstein equation, *Phys. Rev. Lett.*, 122(13), 136001.

Galib, M., Baer, M. D., Skinner, L. B., Mundy, C. J., Huthwelker, T., Schenter, G. K., Benmore, C. J., Govind, N., and Fulton, J. L., 2017, Revisiting the hydration structure of aqueous Na^+. *J. Chem. Phys.*, 146(8), 084504.

Gao, H., Tang, K., Xiao, J. Guo, X., Chen, W., Liu, H., and Wang, G., 2022, Recent advances in "water in salt" electrolytes for aqueous rechargeable monovalent-ion (Li^+, Na^+, K^+) batteries, *J. Energy Chem.*, 69, 84–99.

Guzmán-González, G., Alvarez-Tirado, M., Olmedo-Martínez, J. L., Picchio, M. L., Casado, N., Forsyth, M., and Mecerreyes, D., 2023, Lithium Borate Ionic Liquids as Single-Component Electrolytes for Batteries, *Adv. Energy Mater.*, 13(1), 2202974.

Han, K. S., Yu, Z., Wang, H., Redfern, P. C., Ma, L., Cheng, L., Chen, Y., Hu, J. Z., Curtiss, L. A., Xu, K., Murugesan, V., and Mueller, K. T., 2020, Origin of unusual acidity and Li^+ diffusivity in a series of water-in-salt electrolytes, *J. Phys. Chem. B*, 124(25), 5284–5291.

Head-Gordon, T. and Hura G., 2002, Water structure from Scattering Experiments and Simulation, *Chem. Rev.*, 102(8), 2651–2670.

Hu, G., Yang, Z., Zhang, X., Liu, Y., Lin, Y., Chen, S., Chen, Y., Sa, B., and Zhang, Y., 2024, Strongly solvating triglyme-based electrolyte realizes stable lithium metal batteries at high-voltage and high-temperature. *Energy Storage Mater.*, 69, 103402.

Huang, Y., Zhao, L., Li, L., Xie, M., Wu, F., and Chen, R., 2019, Electrolytes and electrolyte/electrode interfaces in sodium-ion batteries: from scientific research to practical application, *Adv. Mater.*, 31(21), 1808393.

Humphrey, W., Dalke, A., Schulten, K., 1996, VMD: visual molecular dynamics, *Journal of molecular graphics*, 14(1), 33–38.

Hoover, W. G., 1985, Canonical dynamics: equilibrium phase-space distributions, *Phys. Rev. A: At., Mol., Opt. Phys.*, 31, 1695–1697.

Hou, T., Yang, G., Rajput, N. N., Self, J., Park, S., Nanda, J., Persson, K. A., 2019, The influence of FEC on the solvation structure and reduction reaction of $LiPF_6$/EC electrolytes and its implication for solid electrolyte interphase formation, *Nano Energy*, 64, 103881.

Hou, Z., Zhang, X., Ao, H., Liu, M., Zhu, Y., and Qian, Y., 2019, Passivation effect for current collectors enables high-voltage aqueous sodium ion batteries, *Mater. Today Energy*, 14, 100337.

Jensen, K. P., and Jorgensen, W. L., 2006, Halide, ammonium, and alkali metal ion parameters for modeling aqueous solutions, *J. Chem. Theory Comput.*, 2, 1499–1509.

Jeon, J., Lee, H., Choi, J. H., and Cho, M., 2020, Modeling and simulation of concentrated aqueous solutions of LiTFSI for battery applications, *J. Phys. Chem. C*, 124(22), 11790–11799.

Joung, I. N., and Cheatham, T. E., 2008, Determination of Alkali and Halide Monovalent Ion Parameters for Use in Explicitly Solvated Biomolecular Simulations, *J. Phys. Chem. B*, 112(30), 9020–9041.

Kartha, T. R. and Mallik, B. S., 2020, Ionic conductance and viscous drag in water-in-salt electrolytes for lithium and sodium ion batteries and supercapacitors, *Mater. Today Commun.*, 25, 101588.

Karunawan, J., Suryadi, P. N., Mahfudh, L., Santosa, S. P., Sumboja, A., and Iskandar, F., 2023, Truncated octahedral shape of spinel $LiNi_{0.5}Mn_{1.5}O_4$ via a solid-state method for Li-Ion batteries, *Energy Fuels*, 37(1), 754-762.

Kistenmacher, H., Popkie, H., and Clementi, E., 1974, Study of the structure of molecular complexes. VIII. Small clusters of water molecules surrounding Li^+, Na^+, K^+, F^-, and Cl^- ions, *J. Chem. Phys.*, 61, 799–815.

Kubisiak, P. and Eilmes, A., 2017, Molecular dynamics simulations of ionic liquid based electrolytes for Na-Ion batteries: effects of force field, *J. Phys. Chem. B*, 121(42), 9957-9968.

Kubisiak, P., Wróbel, P., and Eilmes, A., 2019, Molecular dynamics investigation of correlations in ion transport in MeTFSI/EMIM–TFSI (Me= Li, Na) electrolytes, *J. Phys. Chem. B*, 124(2), 413-421.

Kumar, P. R., Jung, Y. H., Lim, C. H., and Kim, D. K., 2015, $Na_3V_2O_{2x}(PO_4)_2F_{3-2x}$: a stable and high-voltage cathode material for aqueous sodium-ion batteries with high energy density, *J. Mater. Chem. A*, 3, 6271–6275.

Kundu, D., Talaie, E., Duffort, V., and Nazar, L. F., 2015, The emmerging chemistry of sodium ion batteries for electrochemical energy storage, *Angew. Chem.*, 54, 3431–3448.

Kurzweil, P., 2010, Gaston Plante and his invention of the lead-acid battery-the genesis of the first practical rechargeable battery, *J. Power Sources*, 195, 4424–4434.

Lach, J., Wróbel, K., Wróbel, J., Podsadni, P., and Czerwiński, A., 2019, Applications of Carbon in Lead-Acid Batteries: A Review, *J. Solid State Electro.*, 23, 693–705,

Lahmidi, A., Rabii, S., Chtita, S., Kouali, M., Talbi, M., and Errougui, A., 2024, Molecular dynamics simulations and FTIR spectroscopy investigations on the hydration, transport, and dielectric properties of the $NaF_{(aq)}$ system at various concentrations, *Chem. Phys. Impact*, 8, 100400.

Lee, J. M., 2011, Solvent properties of piperidinium ionic liquids, *Chem. Eng. J.*, 172(2-3), 1066-1071.

Leifer, N., Aurbach, D., and Greenbaum, S. G., 2024, NMR studies of lithium and sodium battery electrolytes, *Prog. Nucl. Magn. Reson. Spectrosc.*, 142-143, 1-54.

Li, W., Dahn, J. R., and Wainwright, D. S., 1994, Rechargeable lithium batteries with aqueous electrolytes, *Science*, 264(5162), 1115-1118.

Li, Z., Bouchal, R., Mendez-Morales, T., Rollet, A-L., Rizzi, C., Le Vot, S., Favier, F. Rotenberg, B., Borodin, O., Fontaine, O. and Salanne, M., 2019, Transport properties of Li-TFSI water-in-salt electrolytes, *J. Phys. Chem. B*, 123(49), 10514–10521.

Liu, G., Yang, Y., Lu, X., Qi, F., Liang, Y., Trukhanov, A., Wu, Y., Sun Z., and Lu, X., 2022, Fully active bimetallic phosphide $Zn_{0.5}Ge_{0.5}P$: a novel high-performance anode for Na-ion batteries coupled with diglyme-based electrolyte. *ACS Appl. Mater. Interfaces*, 14(28), 31803–31813.

Liu, J., Li, D., and Liu, X., 2016, A simple and accurate algorithm for path integral molecular dynamics with the Langevin thermostat, *J. Chem. Phys.*, 145(2).

Liu, C., Min, F., Liu, L. and Chen, J., 2019. Hydration properties of alkali and alkaline earth metal ions in aqueous solution: A molecular dynamics study, *Chem. Phys. Lett.*, 727, 31–37.

Lybrand, T. P., and Kollman, P. A., 1985, Water–water and water–ion potential functions including terms for many body effects, *J. Chem. Phys.*, 83(6), 2923–2933.

Lourenço, T. C., Dias, L. G., and Da Silva, J. L. F., 2021, Theoretical investigation of the Na^+ transport mechanism and the performance of ionic liquid-based electrolytes in sodium-ion batteries, *ACS Appl. Energy Mater.*, 4(5), 4444–4458.

Ma, D., Zhu, C., Fu, T., Ma, Y., and Yuan, X., 2021, Synergistic effect of functionalized ionic liquid and alkanolamines mixed solution on enhancing the mass transfer of CO_2 absorption in microchannel, *Chem. Eng. J.*, 417, 129302.

Maeda, S., Kameda, Y., Amo, Y., Usuki, T., Ikeda, K., Otomo,T., Yanagisawa, M., Seki, S., Arai, N., Watanabe, H., and Umebayashi, Y., 2017, Local structure of Li^+ in concentrated ethylene carbonate solutions studied by low-frequency Raman scattering and neutron diffraction with $^6Li/^7Li$ isotopic substitution methods, *J. Phys. Chem. B*, 121, 10979–10987.

Malaspina, T., Colherinhas, G., Weitzner, S. E., Wood, B. C., 2023, Unraveling local structure of salt-in-Water and water-in-salt electrolytes via ab initio molecular dynamics, *J. Mol. Liq*, 383, 122097.

Martínez, L., Andrade, R., Birgin, E. G., and Martínez, J. M., 2009, PACKMOL: A package for building initial configurations for molecular dynamics simulations, *J. Comput. Chem.*, 30(13), 2157-2164.

Messias, A., da Silva, D. A. C., and Fileti, E. E., 2022, Salt-in-water and water-in-salt electrolytes: the effects of the asymmetry in cation and anion valence on their properties, *Phys. Chem. Chem. Phys.*, 24, 336.

Mistry, A., Grundy, L. S., Halat, D. M., Newman, J., Balsara, N. P., and Srinivasan, V., 2022, Effect of solvent motion on ion transport in electrolytes, *J. Electrochem. Soc.*, 169, 040524.

Molinari, N., Mailoa, J. P., Craig, N., Christensen, J., and Kozinsky, B., 2019, Transport anomalies emerging from strong correlation in ionic liquid electrolytes, *J. Power Sources*, 428, 27-36.

Monti, D., Jónsson, E., Palacín, M. R., and Johansson, P., 2014, Ionic liquid based electrolytes for sodium-ion batteries: Na^+ solvation and ionic conductivity, *J. Power Sources*, 245, 630–636.

Nayak, P. K., Yang, L., Brehm, W. and Adelhelm, P., 2018, From lithium-ion to sodium-ion batteries: advantages, challenges, and surprises, *Angew. Chem., Int. Ed.*, 57(1), 102–120.

Perez, P., Lee, W. K., Prohofsky, E. W., 1983, Study of hydration of the Na+ ion using a polarizable water model, *J. Chem. Phys.*, 79, 388-–392.

Peters, J., Buchholz, D., Passerini, S. and Weil, M., 2016, Life cycle assessment of sodium-ion batteries, *Energy Environ. Sci.*, 9(5), 1744–1751.

Ponrouch, A., Marchante, E., Courty, M., Tarascon, J. M., and Palacin, M. R., 2012, In search of an optimized electrolyte for Na-ion batteries, *Energy Environ. Sci.*, 5(9), 8572–8583.

Prasetyo, N., Canaval, L. R., Wijaya, K., and Armunanto, R., 2015, Lithium (I) in liquid ammonia: A quantum mechanical charge field (QMCF) molecular dynamics simulation study, *Chem. Phys. Lett.*, 619, 158-162.

Reber, D., Kühnel, R. S., and Battaglia, C., 2017, High-voltage aqueous supercapacitors based on NaTFSI, *Sustainable Energy Fuels*, 1(10), 2155–2161.

Rezaei, M., Sakong, S., and Groß, A., 2023, Molecular modeling of water-in-salt electrolytes: A comprehensive analysis of polarization effects and force field parameters in molecular dynamics simulations, *J. Chem. Theory Comput.*, 19(17), 5712–5730.

Roe, D. R., and Cheatham, T. E., 2013, PTRAJ and CPPTRAJ: software for processing and analysis of molecular dynamics trajectory data, *J. Chem. Theory Comput.*, 9(7), 3084–3095.

Rosen, M. E., Grant, C. P., and Dallon, J. C., 2021, Mean square displacement for a discrete centroid model of cell motion, *PLoS One*, 16(12), e0261021.

Salomon-Ferrer, R., Case, D.A. and Walker, R.C., 2013, An overview of the Amber biomolecular simulation package, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 3(2), 198–210.

Shakourian-Fard, M., Kamath, G., Smith, K., Xiong, H., and Sankaranarayanan, S. K., 2015, Trends in Na-ion solvation with alkyl-carbonate electrolytes for sodium-ion batteries: insights from first-principles calculations, *J. Phys. Chem. C*, 119(40), 22747–22759.

Shao, Y., Gudia, H., Brandell, D., and Zhang, C., 2022, Transference number in polimer electrolytes: mind the reference-frame gap, *J. Am. Chem. Soc.*, 144(17), 7583–7587.

Shao, Y., and Zhang, C., 2023, Bruce-Vincent transference numbers from molecular dynamics simulations, *J. Chem. Phys.*, 158, 161104.

Shen, Y., Liu, B., Liu, X., Liu, J., Ding, J., Zhong, C., and Hu, W., 2021, Water-in-salt electrolyte for safe and high-energy aqueous battery, *Energy Storage Mater.*, 34, 461–474.

Shimpi, M. R., Rohlmann, P., Shah, F. U., Glavatskih, S., and Antzutkin, O. N., 2021, Transition anionic complex in trihexyl (tetradecyl) phosphonium-bis (oxalato) borate ionic liquid–revisited. *Phys. Chem. Chem. Phys.*, 23(10), 6190–6203.

Singh, N., and Kashyap, H., 2024, Are NaTFSI and NaFSI salt-based water-in-salt electrolytes structurally similar or different?, *J. Phys. Chem. B*, 128, 7615–7626.

Sneha, P. and Doss, C. G. P., 2016, "Molecular Dynamics: New Frontier in Personalized Medicine" in *Advances in Protein Chemistry and Structural Biology*, Ed. Donev, R., Academic Press, Cambridge, MA, USA, pp. 181–224.

Stettner, T., Walter, F. C., and Balducci, A., 2019, Imidazolium-based protic ionic liquids as electrolytes for lithium-ion batteries, *Batteries Supercaps*, 2(1), 55-59.

Stillinger, F. H., Rahman A., 1978, Revised central force potentials for water. *J. Chem. Phys.*, 68(2), 666–670.

Sui, Y., and Ji, X, 2021, Anticatalytic strategies to suppress water electrolysis in aqueous batteries, *Chem. Rev.*, 121(11), 6654—6695.

Suo, L., Borodin, O., Gao, T., Olguin, M., Ho, J., Fan, X., Luo, C., Wang, C. dan Xu, K., 2015, "Water-in-salt" electrolyte enables high-voltage aqueous lithium-ion chemistries, *Science*, 350(6263), 938–943.

Suo, L., Borodin, O., Sun, W., Fan, X., Yang, C., Wang, F., Gao, T., Ma, Z., Schroeder, M., von Cresce, A., Russell, S. M., Armand, M., Angell, A., Xu, K., and Wang, C., 2016. Advanced high-voltage aqueous lithium-ion battery enabled by "water-in-bisalt" electrolyte. *Angew. Chem. Int. Ed.*, 128(25), 7252–7257.

Suo, L., Borodin, O., Wang, Y., Rong, X., Sun, W., Fan, X., Xu, S., Schroeder, M. A., Cresce, A. V., Wang, F., Yang, C., Hu, Y., Xu, and K., Wang, C., 2017, "Water-in-salt" electrolyte makes aqueous sodium-ion battery safe, green, and long-lasting, *Adv. Energy Mater.*, 7(21), 1701189.

Tang, X., Wang, P., Bai, M., Wang, Z., Wang, H., Zhang, M., and Ma, Y., 2021, Unveiling the reversibility and stability origin of the aqueous V_2O_5-Zn batteries with a $ZnCl_2$ "water-in-salt" electrolyte, *Adv. Sci.*, 8, 2102053.

Tang, X., Lv, S., Jiang, K., Zhou, G., and Liu, X., 2022, Recent development of ionic liquid-based electrolytes in lihium-ion batteries, *J. Power Sources*, 542, 231792.

Thorat, A., Chauhan, R., Sartape, R., Singh, M. R., and Shah, J. K., 2024, Effect of K^+ force fields on ionic conductivity and charge dynamics of KOH in ethylene glycol, *J. Phys. Chem. B*, 128(15), 3707–3719.

Tongraar, A., Lieldl, K. R., and Rode, B. M., 1998, Born–Oppenheimer ab Initio QM/MM Dynamics Simulations of Na^+ and K^+ in Water: From Structure Making to Structure Breaking Effects, *J. Phys. Chem., A*, 102, 10340–10347.

Tsimpanogiannis, I. N., Moultos, O. A., Franco, L. F. M., de M. Spera, M. B., Erdős M., Economou, I. G., 2019, Self-diffusion coefficient of bulk and confined water: a critical review of classical molecular simulation studies, *Mol. Simul.*, 45(4-5), 425–453.

Varma, S., and Rempe, S. B., 2006, Coordination numbers of alkali metal ions in aqueous solutions. *Biophys. Chem.*, 124(3), 192–199.

Vogl, T., Menne, S., Kühnel, R. S., and Balducci, A., 2014, The beneficial effect of protic ionic liquids on the lithium environment in electrolytes for battery applications, *J. Mater. Chem. A*, 2, 8258–8265.

Wang, J., Wang, W., Kollman, P. A. and Case, D. A., 2001, Antechamber: an accessory software package for molecular mechanical calculations, *J. Am. Chem. Soc*, 222(1).

Wang, J., Wolf, R. M., Caldwell, J. W., Kollman, P. A., Case, D.A., 2004, Development and testing of a general Amber force field, *J. Comput. Chem.*, 25, 1157–1174.

Wang, F., Fan, X., Gao, T., Sun, W., Ma, Z., Yang, C., Han, F., Xu, K., and Wang, C., 2017, High-voltage aqueous magnesium ion batteries, *ACS Cent. Sci.*, 3, 1121–1128.

Wang, Y., Hao, X., Kang, Y., Dong, M., Fang, Z., Hu, Y., Wang, H., Fan, X., Yan, Y., Ye, Z., and Peng, X., 2023, Enhanced ion conductivity of "water-in-salt" electrolytes by nanochannel membranes, *J. Mater. Chem. A.*, 11(3), 1394–1402.

Wessells, C., Ruffo, R., Huggins, R. A., and Cui, Y., 2010, Investigations of the electrochemical stability of aqueous electrolytes for lithium battery applications, *Electrochem. Solid-State Lett.*, 13(5), A59.

Wu, X., Liu, Z., Huang, S., and Wang, W., 2005, Molecular dynamics simulation of room-temperature ionic liquid mixture of [bmim][BF_4] and acetonitrile by a refined force field. *Phys. Chem. Chem. Phys.*, 7(14), 2771–2779.

Wu, Y., Tepper, H. L., and Voth, G. A., 2006, Flexible simple point-charge water model with improved liquid-state properties, *J. Chem. Phys.*, 124(2), 024503.

Wróbel, P., Kubisiak, P. and Eilmes, A., 2021, MeTFSI (Me = Li, Na) solvation in ethylene carbonate and fluorinated ethylene carbonate: a molecular dynamics study, *J. Phys. Chem. B*, 125(4), 1248–1258.

Wróbel, P., Kubisiak, P., and Eilmes, A., 2021, NaFSI and NaTFSI solutions in ether solvents from monoglyme to poly (ethylene oxide)—a molecular dynamics study, *J. Phys. Chem. B*, 125(36), 10293–10303.

Xu, N., Shi, J., Liu, G., Yang, X., Zheng, J., Zhang, Z., and Yang, Y., 2021, Research progress of fluorine-containing electrolyte additives for lithium ion batteries, *J. Power Sources Adv.*, 7, 100043.

Yang, X., Zhang, B., Tian, Y., Wang, Y., Fu, Z., Zhou, D., Liu, H., Kang, F., Li, B., Wang, C., and Wang, G., 2023, Electrolyte design principles for developing quasi-solid-state rechargeable halide-ion batteries.*Nat. Commun.*, 14(1), 925.

Yao, N., Chen, X., Fu, Z., and Zhang, Q., 2022, Applying classical, *ab initio*, and machine-learning molecular dynamics simulations to the liquid electrolyte for rechargeable batteries, *Chem. Rev.*, 122, 10970–11021.

Yu, Z., Juran, T. R., Liu, X., Han, K. S., Wang, H., Mueller, K. T., Ma, L., Xu, K., Li, T., Curtiss, L. A., and Cheng, L., 2022, Solvation structure and dynamics of $Mg(TFSI)_2$ aqueous electrolyte, *Energy Environ. Mater.*, 5, 295–304.

Yuan, Y., Jiang, X., Wang, X., Chen, N., and Li, S., 2022, Toxicological impacts of excessive lithium on largemouth bass (*Micropterus salmoides*): Body weight, hepatic lipid accumulation, antioxidant defense and inflammation response, *Sci. Total Environ.*, 841, 156784.

Zalosh, R., Gandhi, P., and Barowy, A., 2021, Lithium-ion energy storage battery explosion incidents, *J. Loss Prev. Process Ind.*, 72, 104560.

Zhang, Y., Lewis, N. H. C., Mars, J., Wan, G., Weadock, N. J., Takacs, C. J., Lukatskaya, M. R., Steinrück, H. G., Toney, M. F., Tokmakoff, A. and Maginn, E. J., 2021, Water-in-Salt LiTFSI aqueous electrolytes (1): Liquid structure from combined molecular dynamics simulation and experimental studies, *J. Phys. Chem. B*, 125(17), 4501–4513.

Zhang, Y. and Maginn E. J., 2021, Water-In-Salt LiTFSI Aqueous Electrolytes (2): Transport properties and Li^+ dynamics based on molecular dynamics simulations, *J. Phys. Chem. B*, 125, 13246–13254.

Zhang, Y., Carino, E., Hahn, N. T., Becknell, N., Mars, J., Han, K. S., Mueller, K. T. Toney, M., Maginn, E. J., Tepavcevic, S., 2023, Understanding the surprising ionic conductivity maximum in $Zn(TFSI)_2$ water/acetonitrile mixture electrolytes, *J. Phys. Chem. Lett.*, 14(50), 11393—11399.

Zhu, Z., Jiang, T., Ali, M., Meng, Y., Jin, Y., Cui, Y., and Chen, W., 2022, Rechargeable Batteries for Grid Scale Energy Storage, *Chem. Rev.*, 122(22), 16610–16751.

Zmpitas, J., and Gross, J., 2021, Modified stokes-einstein equation for molecular self-diffusion based on entropy scaling, *Ind. Eng. Chem. Res.*, 60(11), 4453–4459.