

DAFTAR PUSTAKA

- Abdul Ghani, N.A., Anuar, F.H., Ahmad, A., Mobarak, N.N., Shamsudin, I.J., Dzulkpli, M.Z., and Hassan, N.H., 2020, Incorporating 1-butyl-3-methylimidazolium chloride Ionic Liquid into Iota Carrageenan Solid Biopolymer Electrolyte for Electrochemical Devices Application, *Sains Malays.*, 49, 305–313.
- Abraham, K.M., 2020, How Comparable Are Sodium-Ion Batteries to Lithium-Ion Counterparts?, *ACS Energy Lett.*, 5, 3544–3547.
- Borodin, O., Giffin, G.A., Moretti, A., Haskins, J.B., Lawson, J.W., Henderson, W.A., and Passerini, S., 2018, Insights into the Structure and Transport of the Lithium, Sodium, Magnesium, and Zinc Bis(trifluoromethanesulfonyl)imide Salts in Ionic Liquids, *J. Phys. Chem. C*, 122, 20108–20121.
- Canongia Lopes, J.N., Deschamps, J., and Pádua, A.A.H., 2004, Modeling Ionic Liquids Using a Systematic All-Atom Force Field, *J. Phys. Chem. B*, 108, 11250–11250.
- Chang, T.M. and Billeck, S.E., 2021, Structure, Molecular Interactions, and Dynamics of Aqueous [BMIM][BF₄] Mixtures: A Molecular Dynamics Study, *J. Phys. Chem. B*, 125, 1227–1240.
- Filippov, A., Antzutkin, O.N., Arkhipov, V.P., and Gnezdilov, O.I., 2022, Diffusivity of ethylammonium nitrate protic ionic liquid confined in porous glasses, *J. Mol. Liq.*, 356, 1–6.
- Gupta, S. and Sappidi, P., 2023, Understanding the Molecular-Level Structure and Dynamics of Sodium Ions in Water in Ionic Liquid Electrolytes by Molecular Dynamics Simulations, *J. Chem. Eng. Data*, 68, 162–172.
- Hasa, I., Passerini, S., and Hassoun, J., 2016, Characteristics of an ionic liquid electrolyte for sodium-ion batteries, *J. Power Sources.*, 303, 203–207.
- Kapoor, U. and Shah, J.K., 2018, Thermophysical Properties of Imidazolium-Based Binary Ionic Liquid Mixtures Using Molecular Dynamics Simulations, *J. Chem. Eng. Data*, 63, 2512–2521.
- Ke, Q., Gong, X., Liao, S., Duan, C., and Li, L., 2022, Effects of thermostats/barostats on physical properties of liquids by molecular dynamics simulations, *J. Mol. Liq.*, 365, 1–13.

- 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, 9957–9968.
- Kubisiak, P., Wróbel, P., and Eilmes, A., 2021, How Temperature, Pressure, and Salt Concentration Affect Correlations in LiTFSI/EMIM-TFSI Electrolytes: A Molecular Dynamics Study, *J. Phys. Chem. B*, 125, 12292–12302.
- Kubisiak, P., Wróbel, P., and Eilmes, A., 2020, Molecular Dynamics Investigation of Correlations in Ion Transport in MeTFSI/EMIM-TFSI (Me = Li, Na) Electrolytes, *J. Phys. Chem. B*, 124, 413–421.
- 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, 4444–4458.
- Matsumoto, K., Hwang, J., Kaushik, S., Chen, C.Y., and Hagiwara, R., 2019, Advances in sodium secondary batteries utilizing ionic liquid electrolytes, *Energy Environ. Sci.*, 12, 3247–3287.
- McDaniel, J.G., Son, C.Y., and Yethiraj, A., 2018, Ab Initio Force Fields for Organic Anions: Properties of [BMIM][TFSI], [BMIM][FSI], and [BMIM][OTf] Ionic Liquids, *J. Phys. Chem. B*, 122, 4101–4114.
- 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.
- Monti, D., Ponrouch, A., Palacín, M.R., and Johansson, P., 2016, Towards safer sodium-ion batteries via organic solvent/ionic liquid based hybrid electrolytes, *J. Power Sources*, 324, 712–721.
- Mota, J.V.L., Albuquerque, M., Brandell, D., and Costa, L.T., 2023, Exploring structural and dynamical properties of polymer-ionic liquid ternary electrolytes for sodium ion batteries, *Electrochim. Acta*, 461, 1–11.
- Ngo, H.P.K., Planes, E., Iojoiu, C., Soudant, P., Rollet, A.L., and Judeinstein, P., 2022, Transport properties of alkali/alkaline earth cations in ionic-liquid based electrolytes, *J. Ionic Liq.*, 2, 1–23.
- Nguyen, A.G. and Park, C.J., 2023, Insights into tailoring composite solid polymer electrolytes for solid-state lithium batteries, *J. Memb. Sci.*, 675, 1–79.

- Padhi, A.K., Janežič, M., and Zhang, K.Y.J., 2022, Molecular dynamics simulations: Principles, methods, and applications in protein conformational dynamics, *Adv. Protein Chem. Struct. Biol.*, 26, 439–454.
- Pan, H., Hu, Y.S., and Chen, L., 2013, Room-temperature stationary sodium-ion batteries for large-scale electric energy storage, *Energy Environ. Sci.*, 6, 2338–2360.
- Rampal, N., Weitzner, S.E., Cho, S., Orme, C.A., Worsley, M.A., and Wan, L.F., 2024, Structural and transport properties of battery electrolytes at sub-zero temperatures, *Energy Environ. Sci.*, 17, 7691–7698.
- Salvador, M.A., Maji, R., Rossella, F., Degoli, E., Ruini, A., and Magri, R., 2023, Structural and Dynamic Characterization of Li-Ionic Liquid Electrolyte Solutions for Application in Li-Ion Batteries: A Molecular Dynamics Approach, *Batteries*, 9, 1–22.
- Srour, H., Chancelier, L., Bolimowska, E., Gutel, T., Mailley, S., Rouault, H., and Santini, C.C., 2016, Ionic liquid-based electrolytes for lithium-ion batteries: review of performances of various electrode systems, *J. Appl. Electrochem.*, 46, 149–155.
- Verma, A.K., Thorat, A.S., and Shah, J.K., 2024, Estimating ionic conductivity of ionic liquids: Nernst–Einstein and Einstein formalisms, *J. Ionic Liq.*, 4, 1–10.
- Verma, C., Olasunkanmi, L.O., Bahadur, I., Lgaz, H., Quraishi, M.A., Haque, J., Sherif, E.S.M., and Ebenso, E.E., 2019, Experimental, density functional theory and molecular dynamics supported adsorption behavior of environmental benign imidazolium based ionic liquids on mild steel surface in acidic medium, *J. Mol. Liq.*, 273, 1–15.
- Vignarooban, K., Kushagra, R., Elango, A., Badami, P., Mellander, B.E., Xu, X., Tucker, T.G., Nam, C., and Kannan, A.M., 2016, Current trends and future challenges of electrolytes for sodium-ion batteries, *Int. J. Hydrogen Energy*, 41, 2829–2846.
- Vollmayr-Lee, K., 2020, Introduction to molecular dynamics simulations, *Am. J. Phys.*, 88, 401–422.
- Vranes, M., Dozic, S., Djerić, V., and Gadzuric, S., 2012, Physicochemical characterization of 1-butyl-3-methylimidazolium and 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide, *J. Chem. Eng. Data*, 57, 1072–1077.

- Wafi, N.I.B., Daud, W.R.W., Ahmad, A., Majlan, E.H., and Somalu, M.R., 2019, Effect of lithium hexafluorophosphate LiPF₆ and 1-butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide [Bmim][TFSI] immobilized in poly(2-hydroxyethyl methacrylate) PHEMA, *Polymer Bulletin*, 76, 3693–3707.
- Wang, S., Li, Z., Yang, G., Lin, J., and Xu, Q., 2023, Molecular dynamics study of fluorosulfonyl ionic liquids as electrolyte for electrical double layer capacitors, *RSC Adv.*, 13, 29886–29893.
- Wang, T., Su, D., Shanmukaraj, D., Rojo, T., Armand, M., and Wang, G., 2018, Electrode Materials for Sodium-Ion Batteries: Considerations on Crystal Structures and Sodium Storage Mechanisms, *Electrochem. Energy Rev.*, 1, 200–237.
- 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, 10293–10303.
- Xu, L.Y., Alrefaei, Y., Wang, Y.S., and Dai, J.G., 2021, Recent advances in molecular dynamics simulation of the N-A-S-H geopolymer system: modeling, structural analysis, and dynamics, *Constr. Build Mater.*, 276, 1–12.
- Yang, M.Y., Merinov, B. V., Zybin, S. V., Goddard, W.A., Mok, E.K., Hah, H.J., Han, H.E., Choi, Y.C., and Kim, S.H., 2022, Transport properties of imidazolium based ionic liquid electrolytes from molecular dynamics simulations, *Electrochem. Sci. Adv.*, 2, 1–9.
- Yao, N., Chen, X., Fu, Z.-H., 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.
- Zhao, L., Zhang, T., Li, W., Li, T., Zhang, L., Zhang, X., and Wang, Z., 2023, Engineering of Sodium-Ion Batteries: Opportunities and Challenges, *Engineering*, 24, 172–183.
- Zhao, Y., Kang, Y., Wozny, J., Lu, J., Du, H., Li, C., Li, T., Kang, F., Tavajohi, N., and Li, B., 2023, Recycling of sodium-ion batteries, *Nat. Rev. Mater.*, 8, 623–634.
- Zhu, N., Zhang, K., Wu, F., Bai, Y., and Wu, C., 2021, Ionic Liquid-Based Electrolytes for Aluminum/Magnesium/Sodium-Ion Batteries, *Energy Mater. Adv.*, 2021, 1–29.