REFERENCES

REFERENCES

Abe, A., Jernigan, R. L. and Flory, P. J. (1965). Conformational energies of n-alkanes and the random configuration of higher homologs including polymethylene. *Journal of the American Chemical Society, 88,* 631-639.

Abraham, M., Hess, B., van der Spoel, D. and Lindahl, E. (2020). GROMACS Documentation Release 2020.1. *Royal Institute of Technology and Uppala University: Sweden.* https://doi.org/10.5281/zenodo.3685920.

Abraham, K. M., Jiang, Z. and Carroll, B. (1997). Highly conductive PEO like polymer electrolytes. Chemistry of Materials Journal. 9, 1978–19.

Acevedo, O. (2018). Ionic liquid force field parameters (OPLS-2009IL and OPLS-VSIL). (accessed Dec 24, 2019). https://github.com/ orlandoacevedo/IL.

Akten E. D. and Mattice W. L. (2001). Monte Carlo simulation of head-to-head, tail-to-tail polypropylene and its mixing with polyethylene in the melt. *Macromolecules. 34,* 3389–3395.

Allen, M. P. and Tildesley, D. J. (1987). Computer simulation of liquids, *Oxford: Clarendon Press.*

Anogiannakis, S. D., Tzoumanekas, C. and Theodorou, D. N. (2012). Microscopic description of entanglements in polyethylene networks and melts: strong, weak, pairwise, and collective attributes. *Macromolecules. 45*(23)*,* 9475–9492.

Anwar, M. and Schilling, T. (2015). Crystallization of polyethylene: A molecular dynamics simulation study of the nucleation and growth mechanisms. *Polymer. 76,* 307–312.

Balsara, N. P. and Newman, J. (2015). Relationship between steady-state current in symmetric cells and transference number of electrolytes comprising univalent and multivalent ions. *Journal of The Electrochemical Society. 162,* A2720–A2722.

Baschnagel, J., Binder, K., Doruker P., Gusev, A., Hahn, O., Kremer, K., Mattice, W. L., Muller-Plathe, F., Murat, M., Paul, W., Santos, S., Suter, U. W. and Tries, V. (2000). Bridging the gap between atomistic and coarse-grained models of polymers: status and perspectives. *Advances in Polymer Science. 152,* 41–156.

Bocharova, V. and Sokolov, A. P. (2020). Perspectives for Polymer Electrolytes: A View from Fundamentals of Ionic Conductivity. *Macromolecules. 53,* 4141-4157.

Bovey, F. A., Hood, F. P., Anderson, E. W. and Kornegay, R. L. (1967). Polymer nuclear magnetic resonance spectroscopy. XII. The stereoregularity of poly(vinyl chloride) and its dependence on polymerization temperature. *The Journal of Physical Chemistry. 71,* 312.

Boyd, R. H. and KESNER, L. (1981). Conformational properties of polar polymers. I. poly(vinyl chloride). *Journal of Polymer Science. 19,* 375-391.

Brandrup, J. and Immergut, E. H. (2004). Polymer Handbook. John *Wiley and Sons, New York.*

Cadogan, D. F. and Howick, C. J. (2000). Plasticizers. *Kirk-Othmer Encyclopedia of Chemical Technology.*

Capiglia, C., Mustarelli, P., Quartarone, E., Tomasi, C. and Magistris, A. (1999). Effects of nanoscale SiO2 on the thermal and transport properties of solvent-free, poly(ethylene oxide) (PEO)-based polymer electrolytes. *Solid State Ion*. *118*, 73–79.

Carballeira, L., Pereiras, A. J. and Rios, M. A. (1989). Conformational properties of poly(vinyl bromide) and poly(vinyl fluoride). *Macromolecules. 22*(6)*,* 2668–2673.

Chen, C. M. and Higgs, P. G. (1998). Monte-carlo simulations of polymer crystallization in dilute solution. *The Journal of Chemical Physics. 108,* 4305–4314.

Choi, P. and Mattice, W. L. (2004). Molecular origin of demixing, prior to crystallization, of atactic polypropylene/isotactic polypropylene blends upon cooling from the melt. *The Journal of Chemical Physics. 121*(17)*,* 8647-8651.

Choi, U. H., Ye, Y., Salas de la Cruz, D., Liu, W., Winey, K. I., Elabd, Y. A., Runt, J. and Colby, R. H. (2014). Dielectric and viscoelastic responses of imidazolium-

based ionomers with different counterions and side chain lengths. *Macromolecules. 47,* 777– 790.

Cho, J. and Mattice, W. L. (1997). Estimation of long-Range interaction in coarse-grained rotational isomeric state polyethylene chains on a high coordination lattice. *Macromolecules. 30*(3)*,* 637-644.

Clancy, T. C. and Mattice, W. L. (2000). Rotational isomeric state chains on a high coordination lattice: Dynamic Monte Carlo algorithm details. *The Journal of Chemical Physics. 112*(22)*,* 10049–10055.

Correia, D. M., Sabater i Serra, R., Gómez Tejedor, J. A., de Zea Bermudez, V., Andrio Balado, A., Meseguer-Dueñas, J. M. and Costa, C. M. (2018). Ionic and conformational mobility in poly(vinylidene fluoride)/ionic liquid blends: Dielectric and electrical conductivity behavior. *Polymer. 143,* 164–172.

Daniel, T., Hallinan, Jr. and Nitash P. B. (2013). Polymer electrolytes. *Annual Review of Materials Research. 43,* 503-525.

De la Rosa, A., Heux, L., Cavaille J. Y. and Mazeau, K. (2002). Molecular modeling of the mobility of poly(allyl alcohol), PAA, and poly(vinyl alcohol), PVA. *Polymer. 43,* 5665–5677.

Demir, B., Chan, K. Y., Searles, J. and Searles, D. J. (2020). Structural electrolytes based on epoxy resins and ionic liquids: A molecular-level investigation. *Macromolecules. 53,* 7635– 7649.

Dionne P. J., Ozisik, R. and Picu C. R. (2005). Structure and dynamics of polyethylene nanocomposites. *Macromolecules. 38,* 9351–9358.

Dionne, P. J., Picu, C. R. and Ozisik, R. (2006). Adsorption and desorption dynamics of linear polymer chains to spherical nanoparticles: a monte carlo investigation. *Macromolecules. 39*(8)*,* 3089–3092.

Dobrynin, A. V., Colby, R. H. and Rubinstein, M. (1995). Scaling theory of polyelectrolyte solutions. *Macromolecules. 28,* 1859–187.

Doherty, B., Zhong, X., Gathiaka, S., Li, B. and Acevedo, O. (2017). Revisiting OPLS force field parameters for ionic liquid simulations. *Journal of Chemical Theory and Computation. 13,* 6131–6145.

Doruker, P. and Mattice, W. L. (1997). Reverse mapping of coarse-grained polyethylene chains from the second nearest neighbor diamond lattice to an atomistic model in continuous space. *Macromolecules. 30*(18)*,* 5520-5526.

Doruker, P. and Mattice, W. L. (1998). Dynamics of Bulk Polyethylene on a High Coordination Lattice. *Macromolecular Symposia. 133,* 47-70.

Doruker, P. and Mattice, W. L. (1998). Simulation of polyethylene thin films on a high coordination lattice, *Macromolecules. 31,* 1418–1426.

Doruker, P. and Mattice, W. L. (1999). Mobility of the surface and interior of thin films composed of amorphous polyethylene. *Macromolecules. 32,* 194–198.

Ergoz, E., Fatou, J. G. and Mandelkern, L. (1972). Molecular weight dependence of the crystallization kinetics of linear polyethylene. I. experimental results. *Macromolecules. 5,* 147-157.

Esselink, K., Hilbers, P. A. J. and Van Beest, B. W. H. (1994). Molecular dynamics study of nucleation and melting of n-alkanes. *The Journal of Chemical Physics. 101,* 9033–9041.

Feast, W. J. and Munro, H. S. (Eds). (1987). Polymer surfaces and surfaces. *John Wiley and Sons, New York. 33*(12)*,* 2092.

Feng, G., Chen, M., Bi, S., Goodwin, Z. A. H., Postnikov, E. B., Brilliantov, N., Urbakh, M. and Kornyshev, A. A. (2019). Free and bound states of ions in ionic liquids, conductivity, and underscreening paradox. *Physical Review X. 9,* 021024.

Fenton, D. E., Parker, J. M. and Wright, P. V. (1973). Complexes of alkali metal ions with poly(ethylene oxide). *Polymer. 14,* 589.

Flory, P. J. (1969). Statistical Mechanics of Chain Molecules. *Wile, New York.*

Flory, P. J., Sundararajan, P. R. and DeBolt, L. C. (1974). Configurational statistics of vinyl polymer chains. *Journal of the American Chemical Society. 96,* 5015-5024.

Forrest, J. A., Dalnoki-Veress, K., Stevens, J. R. and Dutcher, J. R. (1992). Effect of free surfaces on the glass transition temperature of thin polymer films. *Physical Review Letters. 77*(10)*,* 2002–2005.

Forsyth, M., Porcarelli, L., Wang, X., Goujon, N. and Mecerreyes, D. (2019). Innovative electrolytes based on ionic liquids and polymers for next-generation solid-state batteries. *Accounts of Chemical Research. 52,* 686–694.

Foteinopoulou, K., Karayiannis, N. C., Laso, M. and Kröger, M. (2009). Structure, dimensions, and entanglement statistics of long linear polyethylene chains. *The Journal of Physical Chemistry B. 113,* 442-455.

Fujiwara, S. and Sato, T. (1997). Molecular dynamics simulations of structural formation of a single polymer chain: Bond-orientational order and conformational defects. *The Journal of Chemical Physics. 107,* 613-622.

Fujiwara, S. and Sato, T. (1998). Molecular dynamics simulation of structural formation of short polymer chains. *Physical Review Letters. 80,* 991–994.

Fujiwara, S. and Sato, T. (1999). Molecular dynamics simulation of structure formation of short chain molecules. *The Journal of Chemical Physics. 110,* 9757–9764.

Fujiwara, S. and Sato, T. (2001). Structure formation of a single polymer chain. I. Growth of trans domains. *The Journal of Chemical Physics. 114,* 6455–6463.

Garbassi, F., Morra, M. and Occhiello, E. (1994). Polymer surfaces — from physics to technology. *John Wiley & Sons. Chichester.*

Gee, R. H., Lacevic, N. and Fried, L. E. (2006). Atomistic simulations of spinodal phase separation preceding polymer crystallization. *Nature Materials. 5,* 39-43.

Graham, W. and Watts, D. C. (1970). Non-symmetrical dielectric relaxation behaviour arising from a simple empirical decay function. *Transactions of the Faraday Society. 66,* 80-85.

Haliloglu, T. and Mattice, W. L. (1998). Mapping of rotational isomeric state chains with asymmetric torsional potential energy functions on a high coordination lattice: Application to polypropylene. *The Journal of Chemical Physics. 108*(16)*,* 6989–6995.

Hallinan, D. T., and Balsara, N. P. (2013). Polymer electrolytes. *Annual Review of Materials Research. 43,* 503.

Harmandaris, V. A., Mavrantzas, V. G. and Theodorou, D. N. (1998). Atomistic molecular dynamics simulation of polydisperse linear polyethylene melts. *Macromolecules. 31,* 7934–7943.

Helfand, E. and Tagami, Y. (1972). Theory of surface between immiscible polymers. *The Journal of Chemical Physics. 56,* 3592–3601.

Holbrey, J. and Seddon, K. (1999). Ionic liquids. *Clean Products and Processes. 1,* 223–236.

Humphrey, W., Dalke, A. and Schulten, K. (1996). VMD: Visual molecular dynamics. *14*(1), 33–38.

Hu, W. and Frenkel, D. (2005). Polymer crystallization driven by anisotropic interactions. In: allegra, G. (eds) interphases and mesophases in polymer crystallization III. *Advances in Polymer Science. 191,* 1–35.

Inoue, T., Matsumoto, A. and Nakamura, K. (2013). Dynamic viscoelasticity and birefringence of poly (ionic liquids) in the vicinity of glass transition zone. *Macromolecules. 46*(15), 6104–6109.

Itoh, T., Fujita, K., Uno, T. and Kubo, M. (2017). Polymer electrolytes based on vinyl ethers with various EO chain length and their polymer electrolytes cross-linked by electron beam irradiation. *Ionics. 23,* 257–264.

Jabbari-Farouji, S., Rottler, J., Lame, O., Makke, A., Perez, M. and Barrat, J. L. (2015). Correlation of structure and mechanical response in solid-like polymers. *Journal of Physics: Condensed Matter. 27*(19), 194131.

Jacek Dudowicz, J., Douglas, J. F. and Freed, K. F. (2014). Two glass transitions in miscible polymer blends?. *The Journal of Chemical Physics. 140*(24), 244905.

Jamornsuriya, S. and Vao-soongnern, V. (2022). Molecular simulation of an initial stage of the ordered-structure formation of linear and ring polymers upon cooling from the melts. *Journal of Molecular Liquids. 363,* 119833.

Jang, J. H. and Mattice, W. L. (2000). A monte carlo simulation for the effect of compression on an amorphous polyethylene melt in very thin confined geometry. *Macromolecules. 33*(4), 1467–1472.

Jorgensen, W. L., Maxwell, D. S. and Tirado-Rives, J. (1996). Development and testing of the OPLS All-Atom force field on conformational energetics and properties of organic liquids. *Journal of the American Chemical Society. 118,* 11225-11236.

Karayiannis, N. C., Giannousaki, A. E., Mavrantzas, V. G. and Theodorou, D. N. (2002). Atomistic monte carlo simulation of strictly monodisperse long polyethylene

melts through a generalized chain bridging algorithm. *The Journal of Chemical Physics. 117,* 5465–5479.

Karayiannis, N. C., Mavrantzas, V. G. and Theodorou, D. N. (2002). A novel monte carlo scheme for the rapid equilibration of atomistic model polymer systems of precisely defined molecular architecture. *Physical Review Letters. 88,* 105503.

Kavassalis, T. A. and Sundararajan, P. R. (1993). A molecular-dynamics study of polyethylene crystallization. *Macromolecules. 26,* 4144–4150.

Keith, J. R., Mogurampelly, S., Aldukhi, F., Wheatle, B. K. and Ganesan, V. Influence of molecular weight on ion-transport properties of polymeric ionic liquids. *Physical Chemistry Chemical Physics. 19,* 29134–29145.

Khongvit, P. and Orrasa, N. N. (2020). Functionalized graphenes as nanofillers for polylactide: Moleculsar dynamics simulation study. *Polymer Composites. 41,* 294-305.

Khongvit, P. (2016). A coarse-grained model for polylactide: glass transition temperature and conformational properties. *Journal of Polymer Research. 23,* 139.

Kikkawa, Y., Suzuki, T., Kanesato, M., Doi, Y. and Abe, H. (2009). Effect of phase structure on enzymatic degradation in poly(L-lactide)/Atactic Poly(3-hydroxybutyrate) blends with different miscibility. *Biomacromolecules. 10*(4), 1013–1018.

Kisliuk, A., Bocharova, V., Popov, I., Gainaru, C. and Sokolov, A. P. (2019). Fundamental parameters governing ion conductivity in polymer electrolytes. *Electrochimica Acta. 299,* 191–196.

Kivelson, D., Jr, E. B. W. and Jr, D. R. L. (1960). Microwave spectrum, structure, dipole moment, and nuclear quadrupole effects in vinyl chloride. *The Journal of Chemical Physics. 32,* 205–209.

Ko, M. J., Waheed, M. J., Lavine, M. S. and Rutledge, G. C. (2004). Characterization of polyethylene crystallization from an oriented melt by molecular dynamics simulation. *The Journal of Chemical Physics. 121,* 2823–2832.

Kotelyanskii, M. and Theodorou, D. N. (2004). Simulation methods for polymers. *Marcel Dekker. New York.*

Koyama, A., Yamamoto, T., Fukao, K. and Miyamoto, Y. (2002). Molecular dynamics simulation of polymer crystallization from an oriented amorphous state. *Physical Review E. 65,* 050801.

Koyama, A., Yamamoto, T., Fukao, K. and Miyamoto, Y. (2003). Molecular dynamics studies on polymer crystallization from a stretched amorphous state. *Journal of Macromolecular Science Part B-Physics. 42,* 821–831.

Koyama, A., Yamamoto, T., Fukao, K. and Miyamoto, Y. (2008). Molecular dynamics studies on spatial scale of low energy excitation in a simple polymer system. *Physical Review.* E. 4-7.

Kremer, F. and Schönhals, A. (2003). Broadband Dielectric Spectroscopy. *Springer-Verlag: Berlin.*

Kumar, S. K., Russell, T. P. and Hariharan, A. (1994). Monte carlo simulations of the free surface of polymer melts. *Chemical Engineering Science. 49,* 2899–2906.

Kusinram, C. and Vao-soongnern, V. (2022). A multiscale simulation of amorphous poly(vinyl alcohol). *Materials Today Communications. 30,* 103029.

Lavine, M. S., Waheed, N. and Rutledge, G. C. (2003). Molecular dynamics simulation of orientation and crystallization of polyethylene during uniaxial extension. *Polymer. 44,* 1771-1779.

Lee, K. J. and Mattice, W. L. (1992). Modeling of glassy poly (vinyl chloride) starting from a random model. *Computational and Theoretical Polymer Science. 2,* 55-63.

Lei, Z., Chen, B., Koo, Y.-M. and MacFarlane, D. R. (2017). Introduction: ionic liquids. *Chemical Reviews. 117*(10)*,* 6633–6635.

Li, C., Choi, P. and Sundararajan, P. R. (2010). Simulation of chain folding in polyethylene: A comparison of united atom and explicit hydrogen atom models. *Polymer. 51,* 2803–2808.

Lodge, T. P. and McLeish, T. C. B. (2000). Self-concentrations and effective glass transition temperatures in polymer blends. *Macromolecules. 33*(14)*,* 5278–5284.

Lodge, T. P., Wood, E. R. and Haley, J. C. (2006). Two calorimetric glass transitions do not necessarily indicate immiscibility: The case of PEO/PMMA. *Journal of Polymer Science Part B: Polymer Physics. 44*(4)*,* 756– 763.

Ludovice, P. J. and Suter, U. W. (1992). In computational modeling of polymers. *Bicerano, J., Ed. Marcel Dekker, New York.* 401.

Luo, C. and Sommer, J. U. (2009). Coding coarse grained polymer model for LAMMPS and its application to polymer crystallization. *Computer Physics Communications. 180,* 1382-1391.

Luo, C. and Sommer, J. U. (2011). Growth pathway and precursor states in single lamellar crystallization: MD simulations. *Macromolecules. 44,* 1523-1529.

Luo, C. and Sommer, J. U. (2013). Disentanglement of linear polymer chains toward unentangled crystals. *ACS Macro Letters. 2,* 31-34.

Luo, C. and Sommer, J. U. (2016). Role of thermal history and entanglement related thickness selection in polymer crystallization. *ACS Macro Letters. 5*(1)*,* 30-34.

Luo, C., Kroger, M. and Sommer, J.-U. (2017). Molecular dynamics simulations of polymer crystallization under confinement: ¨Entanglement effect. *Polymer. 109,* 71–84.

Luo, X. B., Liu, H. J. and Paddison, S. J. (2021). Molecular dynamics simulations of polymerized ionic liquids: mechanism of ion transport with different anions. *ACS Applied Polymer Materials Journal. 3,* 141– 152.

Mansfield, K. F. and Theodorou, D. N. (1990). Atomistic simulation of a glassy polymer surface. *Macromolecules. 23,* 4430–4445.

Manthiram, A., Yu, X. and Wang, S. (2017). Lithium battery chemistries enabled by solid-state electrolytes. *Nature Reviews Materials. 2,* 16103.

Mark, J. E. (1972). Random-coil dimensions and dipole moments of vinyl chloride chains. *The Journal of Chemical Physics. 56,* 451-458.

Matsumoto, A., Del Giudice, F., Rotrattanadumrong, F. and Shen, A. Q. (2019). Rheological scaling of ionic-liquid-based polyelectrolytes in ionic liquid solutions. *Macromolecules. 52,* 2759– 2771.

Mattice, W. L. and Suter, U. W. (1994). Conformational Theory of Large Molecules. The Rotational Isomeric State Model in Macromolecular Systems. *Wiley, New York.*

Mavrantza, I. E., Prentzas, D., Mavrantzas, V. G. and Galiotis, C. (2001). Detailed atomistic molecular-dynamics simulation of the orthorhombic phase of crystalline polyethylene and alkane crystals. *The Journal of Chemical Physics. 115,* 3937-3950.

Mavrantzas, V. G. and Theodorou, D. N. (1998). Atomistic simulation of polymer melt elasticity: Calculation of the free energy of an oriented polymer melt. Macromolecules 31, 6310–6332.

Mayo, S. L., Olafson, B. D. and Goddard W. A. (1990). III, DREIDING: A generic force field for molecular simulations. The Journal of Chemical Physics. 94, 8897–8909.

McDaniel, J. G. and Son, C. Y. (2018). Ion correlation and collective dynamics in BMIM/BF4-based organic electrolytes: From dilute solutions to the ionic liquid limit. *The Journal of Physical Chemistry B. 122,* 7154–7169.

Meyer, H. and Mullller-Plathe, F. (2001). Formation of chain-folded structures in supercooled polymer melts. *The Journal of Chemical Physics. 115,* 7807-7810.

Meyer, H. and Mullller-Plathe, F. (2002). Formation of chain-folded structures in supercooled polymer melts examined by MD simulations. *Macromolecules. 35,* 1241-1252.

Mecerreyes, D. (2011). Polymeric ionic liquids: Broadening the properties and applications of polyelectrolytes. *Progress in Polymer Science. 36,* 1629–1648.

Misra, S., Fleming, P. D. and Mattice, W. L. (1995). Structure and energy of thin films of poly-(1,4-cis-butadiene): a new atomistic approach. *Journal of Computer-Aided Materials Design. 2,* 101–112.

Mittal, K. L. (Ed). (1983). Physicochemical aspects of polymer surfaces. *Plenum Press, New York. 1.*

Mittal, K. L. (Ed). (1983). Physicochemical aspects of polymer surfaces, *Plenum Press, New York. 2.*

Mogurampelly, S. and Ganesan, V. (2018). Ion transport in polymerized ionic liquid–ionic liquid blends. *Macromolecules. 51,* 9471– 9483.

Mogurampelly, S., Keith, J. R. and Ganesan, V. (2017). Mechanisms underlying ion transport in polymerized ionic liquids. *Journal of the American Chemical Society. 139,* 9511– 9514.

Muthukumar, M. (2005). Modeling polymer crystallization. *Advances in Polymer Science. 191,* 241.

Nakajima, A. and Kato, K. (1966). Unperturbed chain dimension of poly(vinyl chloride) polymerized at different temperatures. *Die Makromolekulare Chemie. 95,* 52-63.

Nguyen, H. T., Smith, T. B., Hoy, R. S. and Karayiannis, N. C. (2015). Effect of chain stiffness on the competition between crystallization and glass-formation in model unentangled polymers. *The Journal of Chemical Physics. 143,* 144901.

Nicholson, D. A. and Rutledge, G. C. (2016). Molecular simulation of flow-enhanced nucleation in n-eicosane melts under steady shear and uniaxial extension. *The Journal of Chemical Physics. 145,* 244903.

Ohno, H. (2001). Molten salt type polymer electrolytes. *Electrochimica Acta. 46*(10-11), 1407–1411.

Olivier-Bourbigou, H., Magna, L. and Morvan, D. (2010). Ionic liquids and catalysis: recent progress from knowledge to applications. *Applied Catalysis A: General. 373,* 1–56.

Paul, W., Yoon, D. Y. and Smith, G. D. (1995). An optimized united atom model for simulations of polymethylene melts. *The Journal of Chemical Physics. 103,* 1702–1709.

Piorkowska, E. and Rutledge, G. C. (2013). Handbook of Polymer Crystallization. *John Wiley & Sons, New Jersey.*

Poling, B. E., Prausnitz, J. M. and O'Connell, J. P. (2000). Properties of Gases and Liquids 5th Ed. *McGraw-Hill, New York.*

Poling, B. E., Prausnitz, J. M. and O'Connell, J. P. (2002). Properties of Gases and Liquids 5th Ed. *McGraw-Hill, New York.*

Qian, W. J., Texter, J. and Yan, F. (2017). Frontiers in poly (ionic liquid)s: Syntheses and applications. *Chemical Society Reviews. 46,* 1124–1159.

Quartarone, E. and Mustarelli, P. (2011). Electrolytes for solid-state lithium rechargeable batteries: recent advances and perspectives. *Chemical Society Reviews. 40,* 2525-2540.

Ramos, J., Vega, J. F. and Martınez-Salazar, J. (2015). Molecular dynamics simulations for the description of experimental molecular conformation, melt dynamics, and phase transitions in polyethylene. *Macromolecules. 48,* 5016-5027.

Rane, S. S. and Mattice, W. L. (2004). Relative magnitudes of the short-term motions of the cyclic and linear components of a homopolyrotaxane in θ media. *Macromolecules. 37*(18)*,* 7056–7060.

Rane, S. S. and Mattice, W. L. (2005). Structure and internal dynamics of poly(ethylene oxide) catenanes in the melt. *Macromolecules. 38,* 3708–3712.

Ratner, M. A. and Shriver, D. F. (1988). Ion transport in solvent-free polymers. *Chemical Reviews. 88,* 109–124.

Rehahn, M., Mattice, W. L. and Suter, U. W. (1997). Rotational isomeric state models in macromolecular systems. *Advances in Polymer Science.* 131/132.

Reith, D., Meyer, H. and Mu, F. (2001). Mapping atomistic to coarse-grained polymer models using automatic simplex optimization to fit structural properties. *Macromolecules. 35*(7)*,* 2335-2345.

Rigby, D. and Roe, R. J. (1987). Molecular dynamics simulation of polymer liquid and glass. I. Glass transition. *The Journal of Chemical Physics. 87,* 7285–7292.

Rochow, E. T., Coeler, M., Pospiech, D., Kobsch, O., Mechtaeva, E., Vogel, R., Voit, B., Nikolowski, K. and Wolter, M. (2020). In situ preparation of crosslinked polymer electrolytes for lithium ion batteries: a comparison of monomer systems. *Polymers. 12,* 1707.

Saha, S. and Bhowmick, A. K. (2016). Computer simulation of thermo-plastic elastomers from rubber-plastic blends and comparison with experiments. *Polymer. 103,* 233–242.

Sangoro, J. R., Iacob, C., Agapov, A. L., Wang, Y., Berdzinski, S., Rexhausen, H., Strehmel, V., Friedrich, C., Sokolov, A. P. and Kremer, F. (2014). Decoupling of ionic

conductivity from structural dynamics in polymerized ionic liquids. *Soft Matter. 10,* 3536–3540.

Sangoro, J. R., Iacob, C., Naumov, S., Valiullin, R., Rexhausen, H., Hunger, J., Buchner, R., Strehmel, V., Karger, J. and Kremer, F. (2011). Diffusion in ionic liquids: the interplay between molecular structure and dynamics. *Soft Matter. 7,* 1678–1681.

Scott, M. P., Brazel, C. S., Benton, M. G., Mays, J. W., Holbrey, J. D. and Rogers, R. D. (2002). Application of ionic liquids as plasticizers for poly(methyl methacrylate). *Chemical Communications.* 1370–1371.

Shaplov, A. S., Ponkratov, D. O. and Vygodskii, Y. S. (2018). Poly(ionic liquid)s: synthesis, properties, and application. *Polymer Science, Series B. 58,* 73–142.

Sirirak, K. and Vao-soongnern, V. (2023). Molecular simulation for the effect of chain stiffness on polymer crystallization from the melts. *Journal of Molecular Liquids. 387,* 122650.

Sirirak, K. and Vao-soongnern, V. (2023). Molecular simulation of structural properties of polymer blend nanofilms. *Journal of Polymer Research. 30*(1)*,* 46.

Smith, G. D., Jaffe, R. L. and Yoon, D. Y. (1994). Conformational characteristics of poly(tetrafluoroethylene) chains based upon ab Initio electronic structure calculations on model molecules. *Macromolecules. 27,* 3166-3173.

Smith, G. D., Ludovice, P. J., Jaffe, R. L. and Yoon, D. Y. (1995). Conformations of 2,4-dichloropentane and 2,4,6-trichloroheptane and a force field for poly (vinyl chloride) based upon ab Initio electronic structure calculations. *The Journal of Physical Chemistry. 99,* 164-172.

Solc, K. and Stockmayer, W. H. (1971). Shape of random–flight chains. *The Journal of Chemical Physics. 54,* 2756–2757.

Song, J. Y., Wang, Y. Y. and Wan, C. C. (1999). Review of gel-type polymer electrolytes for lithium-ion batteries. *Journal of Power Sources. 77,* 183–197.

Stamm, M. (1992). Polymer surfaces on a molecular scale: comparison of techniques and some examples. *Advances in Polymer Science. 100,* 357.

Sundararajan, P. R. and Kavassalis, T. A. (1995). Molecular dynamics study of polyethylene chain folding: The effects of chain length and the torsional

barrier. Journal of the Chemical Society, Faraday Transactions. 91, 2541–2549.

Takeuchi, H. (1998). Structure formation during the crystallization induction period of a short chain-molecule system: A molecular dynamics study. *The Journal of Chemical Physics. 1095,* 614–5621.

Tarascon, J. M. and Armand, M. (2001). Issues and challenges facing rechargeable lithium batteries. *Nature. 414,* 359-367.

Theodorou, D. H. and Suter, U. W. (1985). Detailed molecular structure of a vinyl polymer glass. *Macromolecules. 18,* 1467–1478.

Thomas, S., Grohens, Y. and Jyotishkumar, P. (2014). Characterization of polymer blends: miscibility, morphology and interfaces. Eds. *Wiley-VCH Verlag: Weinheim, Germany.*

Vao-soongnern, V. and Jamornsuriya, S. (2021). Molecular simulation of structural and surface properties of poly(ethylene-ran-propylene) thin films. *Journal of Polymer Research. 28,* 340.

Vao-soongnern, V. and Mattice, W. L. (2000). Topological effects on static and dynamic properties in an amorphous nanofiber composed of cyclic polymers. *Macromolecular Theory and Simulations. 9,* 570–577.

Vao-soongnern, V., Doruker, P. and Mattice, W. L. (2000). Simulation of an amorphous polyethylene nanofiber on a high coordination lattice. *Macromolecular Theory and Simulations. 9,* 1-13.

Vao-soongnern, V., Ozisik, R. and Mattice W. L. (2001). Monte carlo simulation of the structures and dynamics of amorphous polyethylene nanoparticles. *Macromolecular Theory and Simulations. 10,* 553-563.

Vao-soongnern, V., Sukhonthamethirat, N., Rueangsri, K., Sirirak, K. and Matsuba, G. (2023). Molecular simulation of the structural formation of mono- and bidisperse polyethylene upon cooling from the melts. *Journal of Molecular Liquids. 376,* 121434.

Vao-soongnern, V., Xu, G. and Mattice, W. L. (2004). Structure formation in the crystallization and annealing of tetracontane nanoparticles. *Macromolecular Theory and Simulations. 13*(6)*,* 539-549.

Vao-soongnern, V. (2006). Nanostructure of the interface modified by grafted polymers: a monte carlo simulation. *Journal of Nanoscience and Nanotechnology. 6,* 3977-3980.

Vao-soongnern, V. (2010). Monte carlo simulations of structures and dynamics of cyclic and linear poly(ethylene oxide) melts. *Computational Materials Science. 49*(4)*,* S369–S371.

Vao-soongnern, V. (2014). A multiscale simulation model for poly (ethylene oxide). *Polymer Science Series. 56,* 928–935.

Verho, T., Paajanen, A., Vaari, V. and Laukkanen, A. (2018). Crystal growth in polyethylene by molecular dynamics: The crystal edge and lamellar thickness. *Macromolecules. 51,* 4865–4873.

Waheed, N., Ko, M. J. and Rutledge, G. C. (2005). Molecular simulation of crystal growth in long alkanes. *Polymer. 46,* 8689–8702.

Waheed, N., Lavine, M. S. and Rutledge, G. C. (2002). Molecular simulation of crystal growth in n-eicosane. *The Journal of Chemical Physics. 116,* 2301–2309.

Watanabe, M. and Mizumura, T. (1996). Conductivity study on ionic liquid/polymer complexes. *Solid State Ionics. 86–88,* 353-356.

Welch, P. M. (2017). Examining the role of fluctuations in the early stages of homogenous polymer crystallization with simulation and statistical learning. *The Journal of Chemical Physics. 146,* 044901.

Wichai, S. and Vao-soongnern, V. (2021). A multiscale simulation of amorphous polystyrene. *Journal of Polymer Research. 28,* 109.

Wichai, K. and Vao-soongnern, V. (2021). Monte carlo simulation of molecular and structural properties of random copolymer thin films. *Journal of Molecular Modeling. 27*(10)*,* 301.

Wright, P. V. (1975). Electrical conductivity in ionic complexes of poly(ethylene oxide). *British Polymer Journal. 7,* 319-327.

Xiao, H., Luo, C., Yan, D. and Sommer, J.-U. (2017). Molecular dynamics simulation of crystallization cyclic polymer melts as compared to their linear counterparts. *Macromolecules. 50,* 9796–9806.

Xu, G. and Mattice, W. L. (2001). Study on structure formation of short polyethylene chains via dynamic Monte Carlo simulation. Computational and Theoretical *Polymer Science. 11*(6)*,* 405–413.

Xu, G. and Mattice, W. L. (2002). Monte carlo simulation of the crystallization and annealing of a freestanding thin film of n-tetracontane. *The Journal of Chemical Physics. 116*(5)*,* 2277–2283.

Xu, G., Lin, H. and Mattice, W. L. (2003). Configuration selection in the simulations of the crystallization of short polyethylene chains in a free-standing thin film. *The Journal of Chemical Physics. 119*(13)*,* 6736–6743.

Xu, G., Vao-soongnern, V. and Mattice, W. L. (2002). Similarities and differences in the rapid crystallization induced in n-tetracontane by an instantaneous deep quench of the free-standing nanofiber and free-standing thin film. *Macromolecular Theory and Simulations. 11*(5)*,* 494-500.

Yabe, M., Mori, K., Ueda, K. and Takeda, M. (2019). Development of PolyPreGen software to facilitate the determination of molecular dynamics simulation parameters for polymers. *Journal of Computer Chemistry, Japan International Edition. 5,* 2018-0034.

Yamamoto, T. (2005). Molecular dynamics modeling of the crystal-melt interfaces and the growth of chain folded lamellae. *Advances in Polymer Science. 191,* 37-85.

Yamamoto, T. (2009). Computer modeling of polymer crystallization - Toward computer-assisted materials' design. *Polymer. 50*(9)*,* 1975-1985.

Yamamoto, T. (2013). Molecular dynamics of polymer crystallization revisited: Crystallization from the melt and glass in longer polyethylene. *The Journal of Chemical Physics. 139,* 054903.

Yamamoto, T. (2014). Molecular dynamics in fiber formation of polyethylene and large deformation of the fiber. *Polymer. 54,* 3086-3097.

Yamamoto, T. (2014). Molecular dynamics of crystallization in a helical polymer isotactic polypropylene from the oriented amorphous state. *Macromolecules. 47,* 3192-3202.

Yao, P., Yu, H., Ding, Z., Liu, Y., Lu, J., Lavorgna, M., Wu, J. and Liu, X. (2019). Review on polymer-based composite electrolytes for lithium batteries. *Frontiers in Chemistry. 7,* 522.

Yi, P. and Rutledge, G. C. (2009). Molecular simulation of crystal nucleation in n-octane melts. *The Journal of Chemical Physics. 131,* 134902.

Yi, P. and Rutledge, G. C. (2011). Molecular simulation of bundle-like crystal nucleation from n-eicosane melts. *The Journal of Chemical Physics. 135,* 24903.

Yi, P., Locker, C. R. and Rutledge, G. C. (2013). Molecular dynamics simulation of homogeneous crystal nucleation in polyethylene. *Macromolecules. 46,* 4723-4733.

Yoshizawa-Fujita, M., Ishii, J., Takeoka, Y. and Rikukawa, M. (2021). Oligoether/Zwitterion diblock copolymers: synthesis and application as cathode-coating material for Li batteries. *Polymers. 13,* 800.

Zhang, H., Liu, C., Zheng, L., Xu, F., Feng, W., Li, H., Huang, X., Armand, M., Nie, J. and Zhou, Z. (2014). Lithium bis(fluorosulfonyl)imide/poly(ethylene oxide) polymer electrolyte. *Electrochimica Acta. 133,* 529–538.

Zhang, J., Liang, Y., Yan, J. and Lou, J. (2007). Study of the molecular weight dependence of glass transition temperature for amorphous poly(l-lactide) by molecular dynamics simulation. *Polymer. 48,* 4900-4905.

Zhang, Q., Liu, K., Ding, F. and Liu, X. (2017). Recent advances in solid polymer electrolytes for lithium batteries. *Nano Research. 10,* 4139–4174.

Zhang, S.Y., Zhuang, Q., Zhang, M., Wang, H., Gao, Z.M., Sun, J. K. and Yuan, J. Y. (2020). Poly(ionic liquid) composites. *Chemical Society Reviews. 49,* 1726–1755.

Zhang, Z. J., Lu, Z. Y., Li, Z. S. and Sun, C. C. (2005). Conformational properties of poly (vinyl Fluoride) based upon ab initio electronic structure calculations. *Chemical Physics Letters. 406*(4-6)*,* 504–508.

Zhang, Z., Nasrabadi, A. T., Aryal, D. and Ganesan, V. (2020). Mechanisms of ion transport in lithium salt-doped polymeric ionic liquid electrolytes. *Macromolecules. 53,* 6995– 7008.

Zhang, Z., Wheatle, B. K., Krajniak, J., Keith, J. R. and Ganesan, V. (2020). Ion mobilities, Transference Numbers, and Inverse Haven Ratios of Polymeric Ionic Liquids. *ACS Macro Letters Journal. 9,* 84–89.