Special Issue

Recent Advances in Thermodynamic Modeling of Ionic Liquids for Energy Applications

Message from the Guest Editors

Ionic liquids (ILs) have emerged as transformative materials in chemical engineering due to their low volatility, thermal stability, and tunable nature. A key advancement in the field is the thermodynamic modeling of ILs. This modeling includes the study of phase equilibria and intermolecular forces, encompassing electrostatic interactions (such as charge–charge, dipole–dipole, and hydrogen bonding) as well as non-electrostatic forces (such as hard-sphere interactions and dispersion forces), which are crucial for understanding the ability of ILs to dissolve or interact with specific compounds. The development of equations of state, excess Gibbs free energy models, and quantum mechanical models has been especially important for accurately describing the phase equilibria of ILs in both electrolyte and non-electrolyte solutions. These models are instrumental in correlating and predicting the performance of ILs in energy-related separation processes, including CO2 capture, biofuel production, electrochemical energy storage, and heat transfer and storage, where precise knowledge of thermodynamic properties and phase equilibria of complex fluids is essential.

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