

From ab Initio Inspired to Coarse-grained Models for Aqueous Solutions and Biomolecules



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ABSTRACT: Molecular simulation capabilities and their applications to systems relevant for chemical engineering have progressed very significantly in recent years. For aqueous electrolyte solutions, newly developed algorithms for “collective” properties such as free energies, solubilities, and transport coefficients reveal systematic deficiencies of existing models that can only be remedied by taking into account electronic polarization and charge transfer effects. One highly promising path for developing next-generation models for such systems is to use machine-learning models based on ab initio (quantum mechanical) calculations. I plan to describe recent progress in this area using the “Deep Potential Molecular Dynamics” approach. Biomolecular phase separation has emerged as an organizing principle underlying subcellular organization and controlling many processes in living systems. The time and length scales relevant for phase transitions of biomolecules far exceed those accessible through atomistic simulations, so coarse-grained, physics-oriented models are appropriate. A specific principle of molecular organization turns out to be competition between macroscopic phase separation and formation of finite-size aggregates, which is also relevant for micelle formation by surfactants. Recent work in this area will be presented that suggests that phase separation dominates at the limit of long, disordered chains.