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Molecular Simulation of Hydrothermal Solutions

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We describe molecular dynamics simulations of supercritical water and supercritical aqueous solutions (including alkali halides and HCl) using simple non-polarizable models of water and a new polarizable model for water developed in our research group. We compare the simulation results to neutron diffraction studies. Dilute supercritical aqueous electrolyte solutions are studied by molecular dynamics to develop a microscopic understanding of ion pairing at near-critical and supercritical conditions, to determine the dissociation constant and the equilibrium constant between paired species for comparison to relevant experimental measurements, and to determine the conductance for comparison with experimental measurements. Recent examples of our work are provided in References 1-3.

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