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Force fields for describing the solution-phase synthesis of shape-selective metal nanoparticles YA ZHOU, The Pennsylvania State University, WISSAM AL-SAIDI, University of Pittsburgh, KRISTEN FICHTHORN, The Pennsylvania State University — Polyvinylpyrrolidone (PVP) and polyethylene oxide (PEO) are structure-directing agents that exhibit different performance in the polyol synthesis of Ag nanostructures. The success of these structure-directing agents in selective nanostructure synthesis is often attributed to their selective binding to Ag(100) facets. We use first-principles, density-functional theory (DFT) calculations in a vacuum environment to show that PVP has a stronger preference to bind to Ag(100) than to Ag(111), whereas PEO exhibits much weaker selectivity. To understand the role of solvent in the surface-sensitive binding, we develop classical force fields to describe the interactions of the structure-directing (PVP and PEO) and solvent (ethylene glycol) molecules with various Ag substrates. We parameterize the force fields through force-and-energy matching to DFT results using simulated annealing. We validate the force fields by comparisons to DFT and experimental binding energies. Our force fields reproduce the surface-sensitive binding predicted by DFT calculations. Molecular dynamics simulations based on these force fields can be used to reveal the role of solvent, polymer chain length, and polymer concentration in the selective synthesis of Ag nanostructures.

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