

Abstract Submitted  
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**First-Principles Theoretical Analysis of Doping in II-VI Compound Semiconductor Nanocrystals** TEJINDER SINGH, TRIANTAFILLOS J. MOUNTZIARIS, DIMITRIOS MAROUDAS, Department of Chemical Engineering, University of Massachusetts, Amherst, COMPUTATIONAL MATERIALS MODELING TEAM — Doping of II-VI compound semiconductor nanocrystals allows for precise control of their optoelectronic and magneto-optical properties. Despite the significant progress in the synthesis of doped nanocrystals, the underlying doping mechanisms in colloidal nanocrystals still remain elusive. Using first-principles density functional theory calculations, we have carried out a fundamental quantitative study of semiconductor nanocrystal doping based on the analysis of adsorption and diffusion of dopants on nanocrystal surface facets. We focus on Mn doping of ZnSe and ZnO nanocrystals with characteristic sizes of  $\sim 5$  nm that have polyhedral shapes with well-defined facets. Our surface kinetic growth model takes into account the equilibrium nanocrystal shape, nanocrystal surface facet structure, nanocrystal composition, surfactants in the growth solution, and dopant surface coverage. Our theoretical results are consistent with recent experimental reports on doping efficiencies and provide an explanation for the doping difficulties during nanocrystal growth.

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