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First-Principles Theoretical Analysis of Dopant Adsorption and Diffusion on Surfaces of II-VI Compound Semiconductor Nanocrystals TEJINDER SINGH, T. J. MOUNTZIARIS, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst — We present a first-principles theoretical analysis of dopant adsorption and diffusion on facets of II-VI semiconductor nanocrystal surfaces and discuss its implications for dopant incorporation into growing nanocrystals. We focus on ZnSe nanocrystals with diameters d$\sim$5 nm that have polyhedral shapes with well-defined facets. Using density functional theory calculations, we find that ZnSe(001)-(2$\times$1) is the energetically favorable surface facet for dopant binding, with multiple adsorption sites. We find that the binding energy for Mn adsorption onto various sites of the ZnSe(001)-(2$\times$1) surface increases with increasing dopant surface concentration. This low binding energy at low dopant surface concentration provides an explanation for doping difficulties during nanocrystal growth. In addition, we have analyzed several dopant migration pathways for Mn diffusion on the ZnSe(001)-(2$\times$1) surface and calculated the corresponding activation barriers as a function of dopant surface concentration. We find that Mn atoms can migrate fast along the Se dimer rows. However, Mn migration to a trough site is governed by a high-barrier process that may lead to dopant incorporation into the ZnSe nanocrystal.

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