

Abstract Submitted  
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**First-Principles Theoretical Analysis of Dopant Diffusion on Surfaces of II-VI Compound Semiconductor Nanocrystals** TEJINDER SINGH, T.J. MOUNTZIARIS, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst — We present a detailed analysis of diffusion of dopants (e.g., Mn, Cu) on surfaces of ZnSe nanocrystals and discuss its implications for dopant incorporation into the growing nanocrystals. We focus on nanocrystals with diameters  $d \sim 5$  nm that have polyhedral shapes with well-defined facets. Using first-principles density functional theory calculations, we have studied the dopant diffusion and adsorption mechanisms and obtained the energetics of various possible dopant diffusion pathways. ZnSe(001)-(2 $\times$ 1) is found to be the energetically favorable surface for dopant binding, with multiple adsorption sites. Our results indicate that dopant atoms can migrate with low activation barriers along the Se dimer rows without substantial surface relaxation. Diffusion across the dimer rows is governed by a higher-barrier pathway, which can lead to dopant incorporation into the nanocrystal through strong bonding with the nanocrystal surface at the corresponding adsorption site in the trough between adjacent dimer rows.

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