Abstract Submitted
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Size-dependent properties of Ga- and Al-doped zinc oxide nanocrystals[1] N. SCOTT BOBBITT, MINJUNG KIM, University of Texas at Austin, NOA MAROM, Tulane University, NA SAI, JAMES R. CHELIKOWSKY, University of Texas at Austin — The feasibility of introducing n-type dopants into ZnO, a popular semiconductor for many photovoltaic and optoelectronic applications, suggests the possibility of controlling the carrier concentration in ZnO nanocrystal systems. We use a real-space pseudopotential method constructed within density functional theory to examine the role of Ga and Al dopants in ZnO nanocrystals in the size regime of 0.8 - 1.5 nm. Nanocrystals with both wurtzite and zincblende structures are examined. We find that while the dopants affect the width of the gap slightly, the highest occupied dopant states are nearly degenerate with the lowest empty state of the undoped nanocrystal. We find the spatial distribution of the dopant state quite similar to the lowest empty state, i.e., they are both localized on the central atom of the nanocrystal. We find that the defect formation energy decreases with increasing particle size, suggesting a less favorable formation energy for smaller nanocrystals.

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