Abstract Submitted
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The role of confinement on the diffusion barriers in semiconductor nanocrystals[1] TZU-LIANG CHAN, ALEXEY ZAYAK, University of Texas at Austin, GUSTAVO DALPIAN, Universidade Federal do ABC, JAMES CHELIKOWSKY, University of Texas at Austin — We find that quantum size effects not only play an important role in the electronic properties of defects in semiconductor nanocrystals, but also strongly affect the incorporation of defect atoms into the nanocrystals. In particular, using ab initio methods based on density functional theory, we predict that Mn defects will be energetically expelled to the surface of CdSe and ZnSe nanocrystals, and that the diffusion barrier of a Mn interstitial defect in a CdSe nanocrystal will be significantly lower than that in the bulk. This can be ascribed to the large surface to volume ratio of nanocrystals, which can effectively release the strain during diffusion. By calculating the vibrational spectrum of the CdSe nanocrystal, we estimated the diffusion rate within the nanocrystal. Our results suggest that energetics can play a role in the self purification of small CdSe and ZnSe nanocrystals, as diffusion of the defect atom can readily occur inside such small nanocrystals.

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