

Abstract Submitted
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Can nanocrystals be charge-doped using surface adsorbates?

ALEX KUTANA, STEVE ERWIN, Center for Computational Materials Science, Naval Research Laboratory — We study theoretically the possibility that lead selenide nanocrystals can be doped with electrons or holes by charge transfer from molecules (hydrazine, N_2H_4) adsorbed on their surface. Despite experiments showing that hydrazine adsorption greatly increases the conductivity of PbSe nanocrystal films, our density-functional theory results show no evidence that carriers are directly created by adsorption. Instead, we find that PbSe always remains intrinsic for a variety of hydrazine coverages and PbSe surface orientations. Moreover, analysis of the charge density shows negligible electron transfer from hydrazine to the surface. We tentatively attribute the discrepancy between experiment and theory to extrinsic factors such as surface defects, doping by surface ligands, or dopant activation by hydrazine. For example, we predict that adsorption of acetic acid will create mobile holes in PbSe, and that surface adsorption of lead atoms will result in mobile electrons.

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