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Hydrogen treatment as a detergent of electronic trap states in lead chalcogenide nanoparticles[1] MARTON VOROS, Materials Science Division, Argonne Natl Lab, NICHOLAS BRAWAND, Institute for Molecular Engineering, University of Chicago, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago and Materials Science Division, Argonne Natl Lab — Lead chalcogenide (PbX) nanoparticles are promising materials for solar energy conversion. However, the presence of trap states in their electronic gap limits their usability, and developing a universal strategy to remove trap states is a persistent challenge. Using calculations based on density functional theory, we show that hydrogen acts as an amphoteric impurity on PbX nanoparticle surfaces; hydrogen atoms may passivate defects arising from ligand imbalance or off-stoichiometric surface terminations, irrespective of whether they originate from cation or anion excess.[1] In addition, we show, using constrained density functional theory calculations, that hydrogen treatment of defective nanoparticles is also beneficial for charge transport in films. We also find that hydrogen adsorption on stoichiometric nanoparticles leads to electronic doping, preferentially n-type. Our findings suggest that post-synthesis hydrogen treatment of lead chalcogenide nanoparticle films is a viable approach to reduce electronic trap states or to dope well-passivated films. [1] M. Voros, N. Brawand, G. Galli, to be published in Chemistry of Materials.

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