Abstract Submitted
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First Principles Simulations of Nanoparticle Solids[1] ARIN GREENWOOD, Institute for Molecular Engineering, University of Chicago, MÁRTON VÖRÖS, Institute for Molecular Engineering, University of Chicago; Materials Science Division, Argonne National Laboratory, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago — Nanoparticle solids are gaining popularity as materials for optoelectronic devices such as solar cells [1, 2]. However, there is still much debate regarding the transport regime governing the charge carriers. To date, no comprehensive description of transport mechanisms in nanoparticle solids has been established, and there is a lack of computational studies predicting electron mobilities and transport rates at the *ab initio* level. In order to understand electron transport properties, it is an essential prerequisite to build realistic structural models of nanoparticle solids to use for prediction of electronic structure and eventually transport properties. Here we present Ab Initio Molecular Dynamics simulations of lead chalcogenide nanoparticles and surrounding ligands to extract relevant electronic structure properties for charge transport calculations. We tested the validity of recently observed "band-like" transport [3] by assessing the formation of bands and their dependence on nanoparticle surface structure and ligands.
[1] Crisp, Ryan et al. Scientific Reports, 2014, 5: 9945. [2] Ning, Zhijun et al. Nature Materials, 2014, 13, pp 822-828. [3] Choi, Ji-Hyuk et al. Nano Letters, 2012, 12(5), pp 2631-2638.

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