Abstract Submitted
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Finite temperature properties of nanoparticle solids: ab initio simulations[1] ARIN GREENWOOD, Institute for Molecular Engineering, University of Chicago, MARTON VOROS, Materials Science Division, Argonne National Laboratory, FEDERICO GIBERTI, Institute for Molecular Engineering, University of Chicago, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago; Materials Science Division, Argonne National Laboratory — Semiconducting nanoparticle (NP) solids are promising materials for optoelectronic devices such as solar cells. However, there is still much debate regarding the transport regime governing the charge carriers due to the disorder of NP films, and there is a lack of computational studies predicting electron mobilities and transport rates at the ab initio level. Using Ab Initio Molecular Dynamics [1] simulations and Density Functional Theory calculations, we built realistic finite-temperature models of bare and halide-capped [2] lead chalcogenide nanoparticle solids and used these models to extract relevant electronic structure and optical properties to gain insight about charge transport in these systems. Computed properties include band gaps, polarizabilities and dielectric constants, as a function of capping and NP solid morphologies. [1] www.qboxcode.org [2] M. Voros, N. Brawand and G. Galli, to be published in Chemistry of Materials

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Arin Greenwood
Institute for Molecular Engineering, University of Chicago

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