Abstract Submitted
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Complementary transport channels in Si-ZnS nanocomposites: first principles simulations[1] STFAN WIPPERMANN, Dep. of Chemistry, University of California, Davis, MARTON VOROS, ADAM GALI, Dep. of Atomic Physics, Budapest University of Technology and Economics, Budapest, GERGELY ZIMANYI, Dep. of Physics, University of California, Davis, GIULIA GALLI, Dep. of Chemistry, University of California, Davis — In solar energy conversion devices, nanoparticles (NPs) are often embedded in solid matrices, either crystalline or amorphous. At present a detailed understanding of the influence exerted by the embedding matrix on the absorption of sunlight by the nanoparticle, and the role of the nanoparticle-matrix interface remain elusive. We investigated Si NPs embedded in ZnS, a system that was used as a charge transport layer in recent experiments. A realistic model of the NP-matrix interface was created from ab-initio molecular dynamics simulations. We found that this nanocomposite exhibits complementary transport channels, where electron transport occurs by hopping between NPs and hole transport through the ZnS-matrix. In analogy to Si NPs embedded in SiO2 [1] we found a strong gap reduction and corresponding red-shifted optical absorption, caused by chemical shifts at the NP-matrix interface.

[1] T. Li, F. Gygi, G. Galli, Phys. Rev. Lett. 107, 206805 (2011)

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