Abstract Submitted
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High pressure core structures of Si nanoparticles for solar energy conversion[1] S. WIPPERMANN, Dep. of Chemistry, University of California, Davis, M. VOROS, Dep. of Atomic Physics, Budapest University of Technology and Economics, Budapest, D. ROCCA, Dep. of Chemistry, University of California, Davis, A. GALI, Dep. of Atomic Physics, Budapest University of Technology and Economics, Budapest, G. ZIMANYI, Dep. of Physics, University of California, Davis, G. GALLI, Dep. of Chemistry, University of California, Davis — Multiple exciton generation (MEG) in semiconductor nanoparticles (NPs) is a promising path towards surpassing the Shockley-Queisser limit in solar energy conversion efficiency. Recent studies demonstrate MEG to be more efficient in NPs than in the bulk, including Si [1]. However, the increased efficiencyis observed only on a relative energy scale in units of the gap: quantum confinement (QC) effects believed to be responsible for efficient MEG in NPs, also increase their optical gap, swiftly shifting the MEG threshold beyond the solar spectrum. Device applications require NPs with low gaps despite the QC enhanced Coulomb interaction. We propose that Si NPs with a core structure resembling that of high pressure Si phases, especially Si-III/BC8, exhibit significantly lower optical absorption thresholds than Si-I NPs, while retaining efficient MEG. The existence of such NPs was recently demonstrated [2]. Our predictions [3] are based on density functional and many body perturbation theory calculations of the electronic, optical and impact ionization properties of hydrogenated Si NPs with high pressure core structures. [1] M. Beard, JPCL 2, 1282 (2011); [2] M. Smith et al., JAP 110, 053524 (2011); [3] S. Wippermann et al. (submitted); [4] M. Voros et al. (submitted)

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