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Multiple Exciton Generation in Si Nanoparticles under pressure¹

STEFAN WIPPERMANN, Dep. of Chemistry, University of California (UC), Davis, MARTON VOROS, Dep. of Atomic Physics, Budapest University of Technology and Economics (T&E), DARIO ROCCA, Dep. of Chemistry, UC Davis, ADAM GALLI, Dep. of Atomic Physics, Budapest University of T&E, GERGELY ZIMANYI, Dep. of Physics, UC Davis, GIULIA GALLI, Dep. of Chemistry, UC 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 theoretical and experimental studies demonstrate MEG to be more efficient in semiconductor NPs than in the bulk material [1]. However, the increased efficiency is observed only on a relative energy scale in units of the gap, as the quantum confinement effects believed to be responsible for efficient MEG in NPs also lead to a significant increase of their gap with respect to the bulk. For successful device applications, it is necessary to identify NPs with enhanced MEG rates on an absolute energy scale. We propose that Si nanoparticles with a core structure resembling that of high pressure Si phases may be promising candidates to exhibit enhanced MEG rates on an absolute scale. In the bulk, upon compression the Si gap is reduced and a recent experimental study demonstrated successful fabrication of Si NPs in the BC8 phase. In the present study we investigate the electronic structure and MEG rates of Si NPs made from the beta-tin, R8, BC8 and hexagonal diamond Si phases from first principles.

[1] M. Beard, *J. Phys. Chem. Lett.* 2, 1282 (2011)

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