Abstract Submitted
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Multiple exciton generation in silicon nanoparticles[1] MARTON VOROS, Department of Atomics Physics, Budapest University of Technology and Economics, ADAM GALI, Hungarian Academy of Sciences, Research Institute for Solid State Physics and Optics, DARIO ROCCA, Department Of Chemistry, University of California, Davis, GIULIA GALLI, Department Of Chemistry, Department Of Physics, University of California, Davis, GERGELY ZIMANYI, Department Of Physics, University of California, Davis — Multiple Exciton Generation (MEG) in semiconductor nanocrystals is considered to be a promising path to improve the efficiency of solar energy conversion. Recent experimental and theoretical studies indicate that MEG is more efficient in nanoparticles (NPs) than in the bulk only on a relative energy scales in units of the gap. The primary cause of this is that quantum confinement increases the energy gap substantially in NPs. MEG will be a true breakthrough when nanocrystals are identified whose impact ionization rate is enhanced even on the absolute energy scale. For this search, we calculated impact ionization rates of silicon NPs with diameters up to 2 nm using density functional theory. Our calculations clearly demonstrate that surface reconstruction creates classes of new states at low energies, de facto lowering the NP gap and thus holding the promise of inreasing MEG even on the absolute energy scale. Our calculations include static screening within the random-phase approximation. We show that a full treatment of the transition matrix elements is essential to obtain correct results due their strong energy dependence.

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