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Germanium nanoparticles for solar energy conversion¹ MÁRTON VÖRÖS, Budapest University of Technology and Economics, STEFAN WIPPERMANN, DARIO ROCCA, GIULIA GALLI, University of California - Davis, ADAM GALI, Wigner Research Center for Physics, Hungarian Academy of Sciences, GERGELY ZIMANYI, University of California - Davis — We propose a strategy to enhance the efficiency of solar energy conversion by elemental germanium, by using Multiple Exciton Generation (MEG) in Ge nanoparticles with a ST12 core structure. The latter is the structure of a high pressure phase of solid Ge. MEG is more efficient in bulk Ge in the diamond phase than in several other semiconductors, e.g. Si. In principle it may be further improved at the nanoscale, due to an increased effective Coulomb interaction. However the electronic energy gap of semiconducting nanoparticles may be too large compared to the visible solar spectrum and their density of states (DOS) too low for efficient solar energy conversion. Using ab initio calculations we found that ST12 Ge nanoparticles of $\sim 1-2$ nm exhibit high impact ionization rates and thus presumably efficient MEG, as well as a gap of ~ 2 eV and a sizable DOS in the low energy part of the spectrum. Therefore these nanoparticles appear to be promising materials for solar energy conversion exploiting MEG.

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