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High-pressure Phase Ge nanoparticles and Si-ZnS nanocomposites: New Paradigms to Improve the Efficiency of MEG Solar Cells STEFAN WIPPERMANN, Max-Planck-Institute for Iron Research, Duesseldorf, MARTON VOROS, University of California, Davis, BALINT SOMOGYI, ADAM GALI, Budapest University of Technology and Economics, DARIO ROCCA, Universite de Lorraine, FRANCOIS GYGI, GERGELY ZIMANYI, GIULIA GALLI, University of California, Davis — The efficiency of nanoparticle (NP) solar cells may substantially exceed the Shockley-Queisser limit by exploiting multi-exciton generation. However, (i) quantum confinement tends to increase the electronic gap and thus the MEG threshold beyond the solar spectrum and (ii) charge extraction through NP networks may be hindered by facile recombination. Using *ab initio* calculations we found that (i) Ge NPs with exotic core structures such as BC8 exhibit significantly lower gaps and MEG thresholds than particles with diamond cores, and an order of magnitude higher MEG rates. (ii) We also investigated Si NPs embedded in a ZnS host matrix and observed complementary charge transport networks, where electron transport occurs by hopping between NPs and hole transport through the ZnS-matrix. Such complementary pathways may substantially reduce recombination, as was indeed observed in recent experiments. We employed several levels of theory, including DFT with hybrid functionals and GW calculations.

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