High-pressure Phase Ge nanoparticles and Si-ZnS nanocomposites: New Paradigms to Improve the Efficiency of MEG Solar Cells

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FAN WIPPERMANN, Max-Planck-Institute for Iron Research, Duesseldorf, MAR- 
TON 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 \textit{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 recombina-
tion, as was indeed observed in recent experiments. We employed several levels of 
theory, including DFT with hybrid functionals and GW calculations.