

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**Ab initio theory of impact ionization applied to silicon nanocrystals**<sup>1</sup> MARTON VOROS, Budapest University of Technology and Economics, ADAM GALI, Hungarian Academy of Sciences, Research Institute for Solid State Physics and Optics, DARIO ROCCA, GERGELY ZIMANYI, GIULIA GALLI, UC Davis — Achieving multi exciton generation (MEG) in semiconducting nanocrystals may lead to overcome the well-known Shockley-Queisser limit when building semiconductor-based solar cells. A thorough, theoretical understanding of the experiments that reported MEG in e.g. Si and PbSe nanocrystals, is still missing and could significantly contribute to clarify the several controversial results in the field. Several theoretical and numerical studies have addressed the origin of the MEG formation, mostly supporting an impact ionization mechanism. However, impact ionization rates have only been evaluated for model nanocrystals by using empirical pseudopotentials fitted to bulk properties, and model dielectric functions to describe the screened Coulomb interaction. We present an ab-initio scheme based on Density Functional Theory in a plane-wave pseudopotential implementation that includes static screening within the random-phase approximation. We will discuss how impact ionization rates are affected by the shape and surface structure of few nm Si nanocrystals.

<sup>1</sup>Support from Grant NSF DMR-1035468 is acknowledged.

Adam Gali  
Hungarian Academy of Sciences,  
Research Institute for Solid State Physics and Optics

Date submitted: 23 Nov 2010

Electronic form version 1.4