Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Convergence of density and hybrid functional defect calculations for compound semiconductors[1] STEPHAN LANY, HAOWEI PENG, NREL, DAVID SCANLON, University College London, VLADAN STEVANOVIC, CSM, JULIEN VIDAL, IRDEP, GRAEME WATSON, Trinity College — Recent revisions of defect formation energy calculations based on band-gap corrected hybrid functionals have raised concerns about the validity of earlier results based on standard density functionals, and about the reliability of the theoretical prediction of electrical properties in semiconductor materials in general. We show here that a close agreement between the two types of functionals can be achieved by determining appropriate values for the electronic and atomic reference energies, thereby mitigating uncertainties associated with the choice of the underlying functional.

[1]Supported by DOE-EERE Next Gen PV II within SunShot initiative.

Stephan Lany
NREL

Date submitted: 12 Nov 2013 Electronic form version 1.4