Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

New perspective on formation energies and energy levels of point defects in non-metals HONG ZHU, University of Connecticut, PATRICK RINKE, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, RAMPI RAMPRASAD, University of Connecticut — We propose a powerful scheme to accurately determine the formation energy and thermodynamic charge transition levels of point defects in non-metals. Previously unknown correlations between defect properties and the valence-band width of the defect-free host material are identified allowing for a determination of the former via an accurate knowledge of the latter. These correlations are identified through a series of hybrid density functional theory computations and an unbiased exploration of the parameter space that defines the Hyde-Scuseria-Ernzerhof family of hybrid-functionals. The applicability of this paradigm is demonstrated for point defects in several insulators, including Si, Ge, ZrO_2 and ZnO

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Date submitted: 11 Nov 2011 Electronic form version 1.4