Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

***Atoms in Solids* Perspective on Polarizabilities and van der Waals Coefficients in Semiconductors** GUO-XU ZHANG, ANTHONY M. REILLY, ALEXANDRE TKATCHENKO, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG — The calculation of response properties of solids including their polarizabilities and van der Waals (vdW) coefficients usually requires the knowledge of the full electronic bandstructure. For non-covalently bound solids, such as noble-gas and ionic crystals, atoms-in-solids model can be successfully utilized to define their polarizabilities. Here we critically assess the atoms-in-solids model for covalently-bound solids, ranging from wide-gap ($\sim$10 eV) to narrow-gap ($\sim$1 eV) semiconductors. We model their response by assigning a single quantum harmonic oscillator to every atom, where the parameters of the oscillators are defined as functionals of the electron density, following the Tkatchenko-Scheffler method [1]. The response function is then calculated by solving self-consistent screening equations of classical electrodynamics, without any explicit information about the electronic bandstructure [2]. The calculated polarizabilities and vdW coefficients for 23 semiconductors are compared with TDDFT and experimental benchmark data, revealing an overall agreement within 10%. We demonstrate the crucial role of vdW interactions in the cohesive properties of the 23 semiconductors.

[1] Tkatchenko and Scheffler, PRL (2009);
[2] Tkatchenko, DiStasio, Car, Scheffler, PRL (2012).

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Date submitted: 15 Nov 2013 Electronic form version 1.4