

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

How van der Waals Interactions Influence Cohesive Properties of Non-Metallic Solids GUO-XU ZHANG, ANTHONY M. REILLY, ALEXANDRE TKATCHENKO, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, Germany — Standard semilocal and hybrid density functionals are widely used for studying cohesive properties of covalent, metallic, and ionic materials. Only recently it has been recognized that long-range van der Waals (vdW) interactions, that are missing in all semilocal and hybrid functionals, are important for an accurate description of cohesion in solids. Here we construct a database of 64 solids where reference cohesive properties are obtained from a critical revision of the available experimental data. All-electron DFT calculations with explicit treatment of zero-point vibrations for all cohesive properties are performed using the LDA, PBE, and the empirical meta-GGA M06-L [1] functionals. For 23 semiconductors, we carry out PBE and M06-L calculations with the inclusion of screened long-range vdW energy [2]. We find that PBE is the most systematic from the three employed functionals, and its accuracy is improved by a factor of two after the inclusion of vdW interactions. The LDA functional considerably overbinds for all the studied solids. The M06-L functional describes middle-range correlation better for certain semiconductors and ionic crystals, but fails for heavier semiconductors and metals.

[1] Zhao and Truhlar, JCP (2006).

[2] Tkatchenko, DiStasio, Car, Scheffler, PRL (2012).

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Date submitted: 08 Nov 2012

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