Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

van der Waals Density Functional Theory vdW-DFq for Semihard Materials[1] QING PENG, SUVRANU DE, Rensselaer Polytechnic Institute — There are a large number of materials with mild stiffness, which are not as soft as tissues and not as strong as metals. These semihard materials includes energetic materials, molecular crystals, layered materials, and van der Waals crystals. The integrity and mechanical stability are mainly determined by the interactions between instantaneously induced dipoles, the so called London dispersion force or van der Waals force. It is challenging to accurately model the structural and mechanical properties of these semihard materials in the frame of density functional theory where the non-local correlation functionals are not well known. Here we propose a van der Waals density functional named *vdW-DFq* to accurately model the density and geometry of semihard materials. Using β-cyclotetramethylene tetranitramine as a prototype, we adjust the enhancement factor of the exchange energy functional with generalized gradient approximations. We find this method to be simple and robust over a wide tuning range when calibrating the functional on-demand with experimental data. With a calibrated value $q = 1.05$, the proposed vdW-DFq method shows good performance in predicting the geometries of 11 common energetic material molecular crystals and 3 typical layered van der Waals crystals.

[1]The authors would like to acknowledge the generous financial support from the Defense Threat Reduction Agency (DTRA) Grant HDTRA1-13-1-0025

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Date submitted: 06 Nov 2015 Electronic form version 1.4