Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

**Self-Consistent Density Functional Including Long-Range van der Waals Interactions** NICOLA FERRI, ROBERT A. DISTASIO JR., ROBERTO CAR, MATTHIAS SCHEFFLER, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG, Berlin, Germany and Princeton University, USA — Van der Waals (vdW) interactions are significant for a wide variety of systems, from noble-gas dimers to organic/inorganic interfaces. The long-range vdW energy is a tiny fraction (0.001%) of the total energy, hence it is typically assumed not to change electronic properties. Although the vdW-DF functional includes the effect of vdW energy on electronic structure [1], the influence of "true" long-range vdW interactions is difficult to assess since a significant part of vdW-DF energy arises from short distances. Here, we present a self-consistent (SC) implementation of the long-range Tkatchenko-Scheffler (TS) functional [2], including its extension to surfaces [3]. The analysis of self-consistency for rare-gas dimers allows us to reconcile two different views on vdW interactions: (i) Feynman's view that claims changes in the electron density and (ii) atoms separated by infinite barrier. In agreement with previous work [1], we find negligible contribution from self-consistency in the structure and stability of vdW-bound complexes. However, a closer look at organic/inorganic interfaces reveals notable modification of energy levels when using the SC-TS vdW density functional. [1] Thonhauser et al., PRB (2007). [2] Tkatchenko and Scheffler, PRL (2009). [3] Ruiz et al., PRL (2012).

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Date submitted: 25 Nov 2012 Electronic form version 1.4