

Abstract Submitted
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Electronic Properties of Polarizable Systems with Self-Consistent Interatomic van der Waals Density Functional NICOLA FERRI, Fritz Haber Institute der MPG, ROBERT A. DISTASIO JR., Princeton University, ALBERTO AMBROSETTI, Fritz Haber Institute der MPG, ROBERTO CAR, Princeton University, MATTHIAS SCHEFFLER, ALEXANDRE TKATCHENKO, Fritz Haber Institute der MPG — Ubiquitous long-range van der Waals (vdW) interactions play a fundamental role in the structure and stability of a wide range of systems. Within the DFT framework, the vdW energy represents a crucial, but tiny part of the total energy, hence its influence on the electronic density, $n(\mathbf{r})$, and electronic properties is typically assumed to be rather small. Here, we address this question *via* a fully self-consistent (SC) implementation of the interatomic Tkatchenko-Scheffler vdW functional [1] and its extension to surfaces [2]. Self-consistency leads to large changes in the binding energies and electrostatic moments of highly polarizable alkali metal dimers. For some metal surfaces, vdW interactions increase dipole moments and induce non-trivial charge rearrangements, leading to visible changes in the metal workfunctions. Similar behavior is observed for molecules adsorbed on metals. Our study reveals a non-trivial connection between electrostatics and long-range electron correlation effects. [1] A. Tkatchenko and M. Scheffler PRL (2009). [2] V. G. Ruiz, W. Liu, E. Zojer, M. Scheffler, and A. Tkatchenko PRL (2012).

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