

Abstract Submitted  
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**Electronic Properties of Surfaces and Interfaces with Self-Consistent van der Waals Density Functional** NICOLA FERRI, Fritz-Haber Institute der MPG, Berlin, Germany, ROBERT A. DISTASIO JR., ROBERTO CAR, Princeton University, USA, ALEXANDRE TKATCHENKO, MATTHIAS SCHEFFLER, Fritz-Haber Institute der MPG, Berlin, Germany — The long-range van der Waals (vdW) energy is only a small part of the total energy, hence it is typically assumed to have a minor influence on the electronic properties. Here, we address this question through a fully self-consistent (SC) implementation of the Tkatchenko-Scheffler (TS) density functional [1]. The analysis of TS-vdW<sup>SC</sup> effects on electron density *differences* for atomic and molecular dimers reveals quantitative agreement with correlated densities obtained from “gold standard” coupled-cluster quantum-chemical calculations. In agreement with previous work [2], we find a very small overall contribution from self-consistency in the structure and stability of vdW-bound molecular complexes. However, TS-vdW<sup>SC</sup> (coupled with PBE functional) significantly affects electronic properties of coinage metal (111) surfaces, leading to an increase of up to 0.3 eV in the workfunction in agreement with experiments. Furthermore, vdW interactions visibly influence workfunctions in hybrid organic/metal interfaces, changing Pauli push-back and charge transfer contributions. [1] A. Tkatchenko and M. Scheffler, PRL (2009); [2] T. Thonhauser *et al.*, PRB (2007).

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