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Density-Functional Theory with Screened van der Waals Interactions for the Modeling of Hybrid Inorganic/Organic Systems[1] VICTOR G. RUIZ, WEI LIU, Fritz-Haber-Institut der MPG, EGBERT ZOJER, Institute of Solid State Physics, Graz University of Technology, MATTHIAS SCHEFFLER, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG — The electronic properties and the function of hybrid inorganic/organic systems (HIOS) are intimately linked to their geometry, with van der Waals (vdW) interactions playing an essential role for the latter. Here we show that the inclusion of the many–body collective response of the substrate electrons inside the inorganic bulk enables us to reliably predict the HIOS geometries and energies. Specifically, dispersion-corrected density-functional theory (the DFT+vdW approach) [*PRL* **102**, 073005 (2009)], is combined with the Lifshitz-Zaremba-Kohn theory [*PRB* **13**, 2270 (1976)] for the non–local Coulomb screening within the bulk. Our method (DFT+vdW$^{\rm surf}$) includes both image-plane and interface polarization effects. We show that DFT+vdW$^{\rm surf}$ yields geometries in remarkable agreement ($\approx$ 0.1 Å) with normal incidence x–ray standing wave measurements for the 3,4,9,10–perylene–tetracarboxylic acid dianhydride ($C_{24}H_8O_6$, PTCDA) molecule on Cu(111), Ag(111), and Au(111). Similarly accurate results are obtained for xenon and benzene adsorbed on metal surfaces.

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