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Van der Waals interactions at the molecule-metal interface: PTCDA on Ag(111) LORENZ ROMANER, DMITRII NABOK, PETER PUSCHNIG, Department of Materials Physics, University of Leoben, Franz-Josef-Straße 18, A-8700 Leoben, Austria, EGBERT ZOJER, Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria, CLAUDIA AMBROSCH-DRAXL, Department of Materials Physics, University of Leoben, Franz-Josef-Straße 18, A-8700 Leoben, Austria — A detailed understanding of the processes governing the adsorption of molecules on metallic surfaces is of major interest for the field of molecular electronics. In this context, the molecule 3,4,9,10-perylene-tetracarboxylic acid dianhydride (PTCDA) has been extensively studied on a variety of metallic surfaces and has so gained fundamental, academic importance. The theoretical description of the adsorption is, however, still controversial as standard density functional theory (DFT) does not include van der Waals interactions, which, for PTCDA and many other molecules, yields the dominant binding contribution. We present DFT calculations of PTCDA adsorbed on Ag(111) where a recently developed exchange-correlation functional was adopted to include van der Waals interactions. Adsorption energy and distances, molecular distortions, charge rearrangements and orbital occupancies are discussed in detail.

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