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Importance of Van Der Waals Interaction for Organic Molecule-Metal Junctions PRIYA SONY, PETER PUSCHNIG, DMITRII NABOK, CLAUDIA AMBROSCH-DRAXL, Chair of Atomistic Modelling and Design of Materials, University of Leoben, Franz-Josef-Strasse 18, A–8700 Leoben, Austria — We present *ab-initio* calculations to study the interface energetics of a weakly adsorbed organic molecule on metallic surfaces, which serve as model interfaces relevant for organic electronics. Thereby we focus on the role of the exchange-correlation potential and, in particular, the van der Waals interaction. To this extent the thiophene molecule is relaxed on clean Cu(110) and Cu(110)-(2x1)O, and the adsorption energy corresponding to various positions and orientations of the molecule is calculated on the search for the most favorable adsorption site. The molecule is found to be more strongly bound on the clean Cu(110) surface with an adsorption energy of -0.50 eV, as compared to -0.30 eV on Cu(110)-(2x1)O. Nonlocal correlations, i.e., the van der Waals interaction is found to be solely reponsible for the binding in such weakly bound systems, while the commonly used generalized gradient approximations not only underestimate the adsorption energyy but also provide the wrong physical picture for the binding. The adsorption of thiophene lowers the work function of the metallic substrate due to the formation of surface dipoles while no sizeable charge transfer is found.

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