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Dissecting an organic-metal bond by molecular manipulation CHRISTIAN WAGNER, NORMAN FOURNIER, CHRISTIAN WEISS, RUSLAN TEMIROV, F. STEFAN TAUTZ, Peter Gruenberg Institut (PGI-3), Forschungszentrum Juelich, Germany —
Scanning probe microscopy with a dynamic AFM has been able to answer some fundamental questions of surface science, like the force necessary to move an atom[1]. Recently, we demonstrated the gradual removal of a single 3,4,9,10-perylenetetracarboxylic-dianhydride (PTCDA) molecule from Ag(111) using a dynamic AFM [2]. The continuous force gradient measurement allowed the structural control over the junction. Here, we show how to extract details of the molecule-surface bonding (physisorption, chemisorption, bonding via functional groups) from such an experiment. The importance of a full-fledged simulation of the lifting -including tip oscillation- is emphasized. We point out the necessity of, and fundamental problems related to, a curved tip trajectory. We study PTCDA on Au(111) and Ag(111) and find qualitatively and quantitatively different binding potentials and adsorption energies. The data represents an ideal benchmark for existing and future ab-initio calculations on these systems. Our method should be applicable to various substrate-adsorbate systems and hence has the potential to answer many open questions in the field.
[1] M. Ternes et al., *Science* **319**, 1066 (2008)
[2] N. Fournier et al., *Phys. Rev. B* **84**, 035435 (2011)

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