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【213】Charge Transfer at Metal-Organic Interfaces Promoted by Dielectric Interlayers: a Comparison of Different Organic Molecular Monolayers on the MgO/Ag(100)-Surface

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Metal-organic interfaces are systems of great interest for both fundamental concepts in electronic structure theory and numerous promising technological applications. Recently, it was demonstrated that an insulating interlayer of MgO on an Ag(100) surface does not simply decouple the metal- and organic-layer but actively promotes charge transfer. While this has been shown for the case of pentacene on MgO/Ag(100)[1], it is interesting to further explore the conditions for charge transfer. Different molecular monolayers on the same surface are studied, aiming at revealing trends in terms of the molecule's electron affinity and size. Here, we present DFT calculations for monolayers of pentacene, PTCDA and H2TPP on MgO/Ag(100) and compare our results to experimental findings.
[1] M. Hollerer. ACS Nano 11, 6252-6260(2017)

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