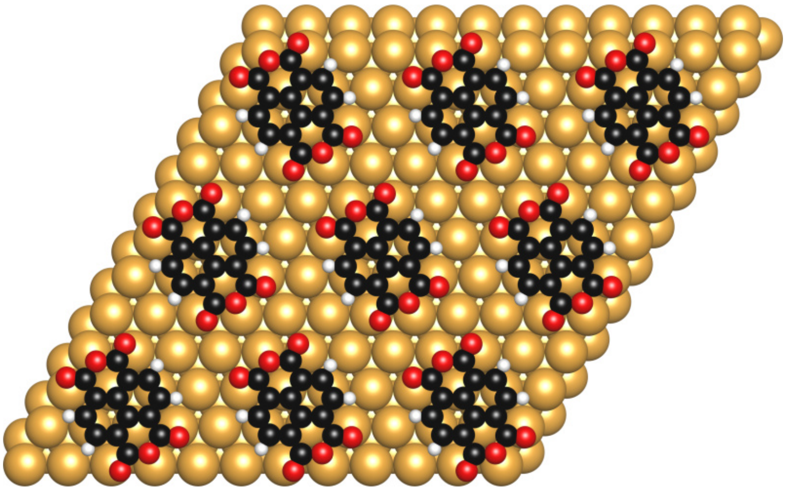
Metal/Organic Interfaces Studied with Density Functional Theory



NTCDA molecules adsorbed on the Au(111) surface.

Introduction

Metal/organic interfaces are found in several technologies that are key to developing modern electronic devices. Examples of such devices include organic light emitting diodes (OLEDs) for displays and efficient solar cells that aim to fulfill the demand for renewable energy.

The interface, where an electron conductor (the metal) and a functional organic material meet, often determines the performance of a device. Yet, many aspects around these interfaces are not fully understood due to the lack of theoretical models.

Methods

Theoretical models are an integral part of unraveling the mysteries of metal/organic interfaces. We employ Density Functional Theory (DFT) to study the atomic structure of interfaces as well as their electronic and optical properties. Since the metallic character is an important aspect that needs to be reproduced, our systems are modeled with the slab approach. While the atomic arrangement is periodically repeated in two dimensions, the third dimension shows a few atomic layers of material and is bordered by a vacuum region.

Results

Depending on their chemical nature, surfaces and molecules can interact in different ways. The less noble a metal, the stronger it will react. Molecules that covalently attach to a surface often change their properties when compared to the gas-phase

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structures. E.g. azulene, which is a flat aromatic molecule, deforms to increase its bonding interaction to the Ag(111) surface while its isomer naphthalene does not [1]. Property changes can be tracked with spectroscopy. Coupling theory with experiment allows one to obtain a detailed understanding of processes taking place at the interface. For a related aromatic molecule, PTCDA, the differences between a mono- and bilayer on Ag(111), were studied [2]. It could be shown that the second layer behaves more like a free-standing layer than the contact layer. In conclusion, the influence of the interface on the properties of the organic bulk materialwas small.

Outlook

The versatility of organic synthesis provides the means to create functionalities which might tune the interface in novel ways. Recent developments include metal-organic hybrid layers and 1D/2D materials. As the library of different molecules increases, theoretical models have to be constantly updated and tested.
In addition we aim to apply bonding analysis schemes to metallic systems.

Publications

Reference

[1] Klein, B. P., van der Heijden, N. J., Kachel, S. R., Franke, M., Krug, C. K., Greulich, K. K., ... & Bocquet, F. C. (2019). Molecular Topology and the Surface Chemical Bond: Alternant Versus Nonalternant Aromatic Systems as Functional Structural Elements. Physical Review X, 9(1), 011030. https://doi.org/10.1103/PhysRevX.9.011030

[2] Zaitsev, N. L., Jakob, P., & Tonner, R. (2018). Structure and vibrational properties of the PTCDA/Ag (1 1 1) interface: bilayer versus monolayer. Journal of Physics: Condensed Matter, 30(35), 354001. https://doi.org/10.1088/1361-648X/aad576

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