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【212】Energy-level Alignment for Tetraphenylporphyrins on Oxide surfaces

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Porphyrin-substrate hybrid systems are the building blocks in a series of materials, such as the organic light-emitting diodes, chemical sensors and dye-sensitized solar cells. Understanding and correctly describing the way molecules interact with the substrate upon adsorption hold the key to the prediction and improvement of the present-day devices.

Recently, distinct features were observed in the photoemission spectra of Co(II)-tetraphenylporphyrin on Mg(100) related to the molecular monolayer and film[1]. Here we investigate the structural and electronic changes the molecule undergoes upon deposition in the framework of hybrid density-functional theory and beyond it. Our simulations of adsorption at different surface sites give an insight into the underlying interaction as compared to the crystal.

[1] Franke et.al., Phys.Chem.Chem.Phys., 2017, 19, 11549-11553

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