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【662】Predicting fundamental gaps of physisorbed one-dimensional acenes

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Experimentalists at Empa recently succeeded in the on-surface synthesis of a variety of open-shell one-dimensional acenes. Their electronic spectra were obtained by means of scanning tunneling spectroscopy for molecules physisorbed on noble metal substrates. Comparison to theoretical predictions requires a proper treatment of the image charge effect in the renormalization of molecular energy levels at the surface compared to the gas phase. We discuss a method for a self-consistent update of molecular gas-phase single-particle wavefunctions due to the image-charge effect. It turns out that this update is crucial even for a qualitative prediction of fundamental gaps of physisorbed acenes on noble metal substrates.

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