Towards Chemical Accuracy for Molecule-Surface Interactions

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A hybrid method is presented[1] that combines MP2 on cluster models with DFT+dispersion on periodic models (plus ΔCCSD(T) corrections) and yields binding energies of molecules on (simple) metal oxide surfaces with chemical accuracy. Examples are the binding of CO and CH_4 on Mg(001),[2] of H_2, CH_4, CO and CO_2 on the internal surfaces of metal organic frameworks (MOF),[3-5] as well as the adsorption and conversion of hydrocarbons in zeolites.[6,7] For comparison with experiments, zero-point vibrational energy contributions are important.

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