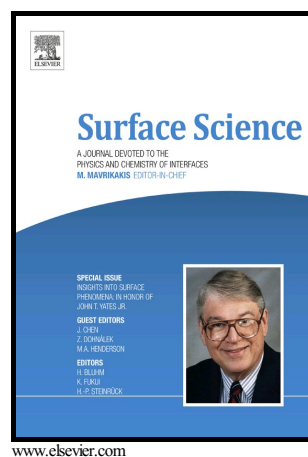


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CO-Decorated Rutile-Type $\text{ZnF}_2(110)$: A Periodic DFT Study

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CO-Decorated Rutile-Type $\text{ZnF}_2(110)$: A Periodic DFT Study

ACCEPTED MANUSCRIPT

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Abstract

Weak binding of small molecules onto surfaces is a powerful tool whereby interfacial phenomena can be studied in atomistic level. It is well-recognized that physisorption is a precursor to chemisorption and the subsequent heterogeneous catalysis. Although at least in part overlooked, vdW-driven sorption of particles on rutile-like substrates is of potential value due to the wide variety of the applications it serves. Probing the acidity of rutile-structured adsorbents by means of carbon monoxide adsorption is the quintessential case of long-range-dominated adsorption on such materials. Monomer, half-layer and monolayer physisorption of gaseous CO at (110) facet of rutile-like ZnF_2 was investigated through dispersion free and dispersion-corrected DFT. Commensurate with the pertinent literature, the upright C-ligated monomer when bound to unsaturated Zn, was found to be energetically favored over the O-ligated conformer. The PBE and optB88-vdW calculated stretching frequencies for freestanding and adsorbed CO were in excellent agreement with their experimentally observed counterparts. Traditional vdW-DF and its successor, vdW-DF2, predict surface energies that match well with B3LYP result. As well, outstanding consistency was found between the vdW-DF and vdW-DF2 computed binding energies and their highly accurate LMP2 equivalent. Whilst being computationally far more efficient, vdW-DF and vdW-DF2 attained interaction energies were closer to the LMP2 benchmark data than the previously reported B3LYP adsorption energy.

Keywords: *Atomic displacements, adsorption energy, dispersion-corrected DFT, CO, rutile, ZnF_2 .*

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