

Probing the (110)-Oriented Plane of Rutile ZnF₂: A DFT Investigation

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Abstract

For many years, rutile-like crystals have given rise to pronounced enthusiasm amongst mineralogists. In this context, rutile-type ZnF₂ has found numerous applications across a variety of disciplines, ranging from material sciences to optoelectronics. Surprisingly, very limited literature is concerned with the molecular adsorption on ZnF₂ surfaces and their related energetics. Additionally, surface probing with small particles is a well-entrenched technique to analyze the interfacial properties. In this regard, small organic species are valuable picks. In the present work, we have employed electronic structure calculations to simulate the adsorption of methane, chloroform, pyrrole, benzene, naphthalene, anthracene, tetracene and pentacene at the (110) plane of rutile ZnF₂. A dispersion-corrected DFT method was chosen to predict the binding energies and structures of molecule-adsorbed surfaces. Interestingly, a linear proportionality relationship was found between the binding energies of aromatic adsorbates and their respective molecular lengths. By applying this correlation, we were able to predict the adsorption energy of pentacene on ZnF₂ to within 2% of our DFT-based result.