A Theoretical Study of Copper Adsorption on the (110) Surface of TiO_2

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Strong interactions between metal catalysts and their supporting oxide substrates give rise to enhanced catalytic properties. Using Density Functional Theory, we are exploring this phenomenon for the prototypical system of copper on the (110) surface of rutile TiO_2. In this poster, we will present our results for the first stages of this investigation, including predictions of the optimal binding site and binding energy for Cu at various coverages on the stoichiometric (110) surface of TiO_2. Connections will be drawn to recent experiments, and an overview of our ongoing investigations will be presented.