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Structure, Energetics, and Clustering Interactions for Cu on TiO_2 (110) at Various Coverages SCOTT J. THOMPSON, STEVEN P. LEWIS, University of Georgia — TiO_2 (110) is one of the prototypical metal-oxide surface systems, studied extensively and under a variety of different conditions by experimentalists and theorists alike. Recent experiments have enhanced our understanding of the structure of the stochiometric surface, and our Density Functional Theory calculations show excellent quantitative agreement with these latest results. In addition, strong interactions between metal catalysts and their supporting oxide substrates give rise to enhanced catalytic properties, and we are exploring this phenomenon for the prototypical system of Cu on the (110) surface of rutile TiO_2. In this talk, we will present our theoretical results for the surface structure and elaborate on the agreement with the latest experimental findings as well as the differences from previous theoretical work on this important system. We will also discuss predictions of the structure and energetics for Cu on TiO_2 (110) at various coverages and on both stoichiometric and reduced surfaces, where specific focus will be upon clustering interactions and the formation of Cu islands, which has been observed experimentally.

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