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The Onset of Ordered Vacancy Configurations on the TiO_2 (110) Surface. SCOTT J. THOMPSON, STEVEN P. LEWIS, University of Georgia — The (110) surface of TiO_2 is a prototypical metal-oxide surface system that has numerous important industrial applications relating to solar energy, gas sensors, and the decomposition of harmful organic compounds. Extensive experimental and theoretical studies have shown that the most common surface defects, bridging O vacancies, play an important role in the desired oxidation processes of this model photocatalyst. Additionally, experimentally observed surfaces have shown the tendency for these defects to arrange themselves in both isolated and highly ordered configurations at low and high vacancy concentrations, respectively. Through Monte Carlo simulations of a converged cluster-expansion model parameterized by density functional calculations, we have observed the onset of multiple ordered configurations of bridging oxygen vacancies at different concentrations. In this talk, we will present our results that show two long-ranged ordered configurations over a relatively wide range of chemical potentials in addition to two semi-ordered configurations, all of which are in good qualitative agreement with experimental and theoretical results.

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