INFRARED PHOTODISSOCIATION CLUSTER STUDIES ON CO_2 INTERACTION WITH TITANIUM OXIDE CATALYST MODELS

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Titanium oxide catalysts are some of the most promising photocatalyst candidates for renewable energy storage applications via production of solar fuels. To contribute to a molecular-level understanding of the interaction of CO_2 with titanium oxide, we turn to cluster models in order to circumvent the challenges posed by speciation in the condensed phase. In this work, we use infrared photodissociation spectroscopy ($950 - 2400$ cm^{-1}) in concert with density functional theory calculations to identify and characterize $[TiO_x(CO_2)_y]^-$ ($x = 1 - 3$, $y = 3 - 7$) clusters. We use these model systems to study the interaction of CO_2 with TiO, TiO_2, and TiO_3, and we find that each species exhibits unique infrared signatures and binding motifs. We will discuss the structures of these cluster ions, and how the coordination of the titanium atom plays a role in reduction of CO_2.