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Conversion of CO2 into Useful Fuels using Cux/TiO2Photocatalysts[1] SATISH KUMAR IYEMPERUMAL, AARON N. DESKINS, worcester polytechnic institute, NA TEAM — Conversion of carbon dioxide, an abundant greenhouse gas, into useful fuels can help solve issues associated with both energy and the environment. Experiments have successfully shown activity for CO_2 conversion to products like methanol using Cu/TiO_2 photocatalysts. How this catalyst works and how it could be improved is an area of much research. We studied this catalyst using density functional theory (DFT) to obtain atomic level insights in the CO_2 reduction process on the catalyst surface. A key activation step in CO2 reduction is the formation of CO_2 anion species with a bent structure. We modeled small Cu_x (x=1-4) clusters on a TiO_2-anatase surface. Our results show that Cu is able to activate CO_2 into a bent configuration that can be further reduced. Charge analysis indicates that CO_2 does indeed become negatively charged in a bent configuration, but not in a linear adsorption mode. We analyzed charge on Cu to assign its oxidation state, as well as calculating adsorbed CO vibrational modes, a common experimental method to assign oxidation state of supported metals. Our results identify how Cu clusters on TiO_2 surfaces may activate CO_2. Such knowledge is crucial towards refining and designing better catalysts for CO_2 reduction.

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