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Modeling Chemical Reactions on Metal Oxide Surfaces[1] HAITAO LIU, University of Pittsburgh, MICHAEL FALCETTA, Grove City College, KENNETH JORDAN, University of Pittsburgh — Photocatalytic conversion of carbon dioxide to methanol has been observed at titanium dioxide interfaces, but the detailed mechanisms are unknown. Computer simulations can prove valuable in elucidating the mechanisms and aid in improving the efficiency. Two major computational strategies for treating such systems are slab and cluster models. The present work uses both periodic slab and embedded cluster models to elucidate the important factors in developing an embedding scheme that properly treats the system and allows the treatment of excited electronic states. Ground state adsorption energies are calculated for a variety of basis sets, cluster sizes, electronic structure methods and embedding schemes to demonstrate convergence with respect to all of these variables. Detailed comparisons of the electrostatic potential obtained from periodic and embedded cluster models are presented to clarify the importance of various effects in the embedding scheme.

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