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First principles study of the activation of carbon dioxide on catalytic surfaces SUJATA PAUL, MARCO BUONGIORNO-NARDELLI, NC State University — Using calculations from first principles we have elucidated the atomic scale mechanisms of activation and reduction of carbon dioxide on specifically designed catalytic surfaces. Among the many reactions that require the development of novel catalytic materials, the understanding of adsorption, activation and reduction of carbon dioxide (CO_2) has become central to the effort to manage greenhouse gas emission and control, if not revert, global warming. In this work we will show how one can use first-principles calculations based on Density Functional Theory to design catalytic surfaces specifically tailored for the activation and reduction of carbon dioxide via the rational manipulation of the surface properties that can be achieved by combining transition metal thin films on oxide substrates. The mechanisms of the molecular reactions on the class of catalytic surfaces so designed will be analyzed in an effort to optimize materials parameters in the search of optimal catalytic materials.

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