

# Physics Colloquium

Michigan Technological University

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Room 139 Fisher Hall



## First-principles Studies of CO<sub>2</sub> Photo-reduction on Titanium Oxide

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**Abstract:** An attractive alternative to photovoltaic cells is to convert and store solar energy in the form of chemical bonds, which involves the photosynthetic production of reduced fuels, such as CH<sub>4</sub> and CH<sub>3</sub>OH. The ‘direct’ conversion of light energy to chemical energy by reduction of CO<sub>2</sub> is anything but ‘direct’ in terms of theoretical understanding of reaction mechanisms. Titania-based photocatalysts are among the most widely studied systems and while CO<sub>2</sub> reduction has been observed on these photocatalysts, the reaction efficiencies are generally very low. The lack of catalysts that can use photoexcited electrons to rapidly cleave C–O bonds in carbon dioxide is the major obstacle for its efficient conversion into energy-bearing products.

We have carried out first-principles calculations to explore reaction mechanisms of CO<sub>2</sub> reduction to HCOOH or CO catalyzed by anatase (101) surface and to provide input for design of new catalysts. Two energetically competitive reaction pathways to HCOOH were identified. Based on the determined rate-limiting step, we have carried out screening of substitutional surface cation doping and found metallic elements that could substantially lower the reaction barriers. A simple model describing the relationship between the activation barriers and the binding energies of CO<sub>2</sub><sup>-</sup> to the dopant surface site is proposed.

**Bio:** Dr. Zapol is a physicist at Argonne National Laboratory. He received his BS and MS from Latvian State University and PhD from Michigan Tech. His research is focused on the computational studies of materials aimed at understanding their structures and physical properties. The majority of this research exploits quantum mechanical methods and molecular dynamics to studies of interactions of molecules with surfaces, interfacial structures, carbon and oxide nanomaterials. Zapol is actively pursuing projects in catalysis, synthesis, energy storage and other energy-related fields.

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