

## Organic Hydride-Catalyzed Reduction of CO<sub>2</sub> to Methanol via Hydride/Proton Transfer Steps

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Conversion of carbon dioxide to fuels enabling a closed-carbon cycle powered by recyclable energy has the potential to dramatically impact the energy and environmental fields, and accordingly has received very considerable experimental and theoretical attention. In this talk, we will describe quantum chemical calculations--- ultimately inspired by the experimental discovery of the efficient photoelectrochemical catalytic reduction of CO<sub>2</sub> to CH<sub>3</sub>OH by some pyridine-derived catalyst---of a homogeneous pathway for this reaction. Our results indicate that this pathway involves the production of the hydride donor 1,2-dihydropyridine PyH<sub>2</sub>, a 2H<sup>+</sup>/2e<sup>-</sup> transfer product of pyridine (Py), which acts as a powerful recyclable organo-hydride that reduces CO<sub>2</sub> to CH<sub>3</sub>OH via three hydride and proton transfer steps. The coupled (or uncoupled) character of these steps, the driving force for them, and the roles of the absorbed light, the cathode, and proton relays in the aqueous solvent will also be discussed.