Tuesday, January 22, 2019, 12:30 pm
Seaver Science Library, Room 150
SSC Auditorium next to the library

Dr. Aaron Appel

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Using Free Energies for H+ and H– Transfers to Design Catalysts for the Reduction of CO_2

The free energies for individual bond forming and bond breaking events can be used to design catalysts for a variety of transformations. In enzymes, catalytic intermediates are closely matched in energy, which provides inspiration for the design of catalysts that can avoid large mismatches in energy throughout the catalytic cycle. While this general approach has been extensively used for designing catalysts for hydrogen production and oxidation, it is equally valuable for the production and use of fuels based on carbon. The utilization of inexpensive substrates such as CO_2 provides an opportunity for large-scale energy storage, and in particular, CO_2 can potentially be converted to liquid fuels for transportation. However, these multistep transformations require efficient catalysts to enable the interconversion of energy and fuels. By matching the free energies for each step in catalytic transformations, we have designed molecular catalysts based on first-row transition metal complexes for the hydrogenation of CO2 to formate, both in traditional organic solvents and in aqueous solutions.

Hosted by Professor Smaranda Marinescu

The scientific community is invited

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