



Insights from Simulations of Sum Frequency Generation Spectroscopy of CO₂-Reduction Catalysts

WHO? Ben Rudshiteyn, Friesner Group

WHEN? Wednesday, March 13th, 2019 at 5:15 pm

WHERE? 7th Floor Lounge, 711 Havemeyer

ABSTRACT I will discuss one of my PhD projects (Yale University, Batista Group) involving the investigation of the surface interactions of the CO₂-reduction catalyzed by the ReI(bpy)(CO)₃Cl complex. My role involved using density functional theory, ab initio molecular dynamics, and time-dependent perturbation theory to help interpret vibrational sum frequency generation (Lian group, Emory) and electrochemical (Kubiak group, UCSD) measurements in collaboration with Maurer at Warwick. We found that the catalyst functionalized with cyano groups binds to a gold surface in such a way as to leave the Cl exposed to the environment and to allow electron-hole-pair coupling-induced vibrational energy transfer. We also found that the catalyst functionalized with carboxyl groups binds to anisotropic rutile TiO₂ in an anisotropic way. I will cover the problem of simulating vibrational sum frequency generation spectroscopy as a pedagogical concept.

Plenty of pizza will be provided.