Explorations of the Synthesizability and Photoelectrochemical Properties of Metastable Semiconductors

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Chemistry Seminar on *Photo-electrochemistry*

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Abstract: Metastable semiconductors have been discovered in many chemical systems that have desirable properties for driving fuel-producing redox reactions from sunlight, including broad visible-light absorption, optimal band edge energies, defect tolerance, and functional carrier mobilities. These photoelectrochemical properties have frequently been found to stem from their metastable nature, e.g., specific features in their crystalline structures and/or compositions lead to being thermodynamically unstable with respect to phase segregation. Recent results will be presented on mixed-metal oxides and carbon nitrides that demonstrate new flux-mediated syntheses and kinetic stabilization in this growing class of semiconductor systems.[1-3] Their syntheses have been achieved by reactions that leverage the exothermic formation of stable salt side products as well as shortened reaction diffusion pathways and low reaction temperatures. Kinetic stabilization of the products has also been enhanced via the application of a) high cohesive energies of an underlying substructure that is maintained during the reaction, and b) solid solution compositions which help to inhibit phase segregation while also providing for percolation pathways. These approaches have yielded, e.g., the first known Sn(II)-perovskites that are isoelectronic to widely commercialized Pb(II)-containing piezoelectrics. Photocatalytic properties in these systems will primarily be described for light-driven H_2O and CO_2 reduction as polycrystalline films and as suspended powders when in aqueous solutions under ultraviolet and visible-light irradiation.

References:

1) *Capturing Metastable Oxide Semiconductors for Applications in Solar Energy Conversion.* Maggard, P.A. *Acc. Chem. Res.* **2021**, *54*, 3160-3171.

2) *Unveiling the Complex Configurational Landscape of the Intralayer Cavities in a Crystalline Carbon Nitride*. Maggard, P.A. et al. *Chem. Sci.* **2022**, *13*, 3187-3193.

3) Renaissance of Topotactic Ion-Exchange for Functional Solids with Close Packed Structures. Maggard, P.A. et al. *Chem. Eur. J.* **2022**, *28*, e202200479(1-6).

About the speaker: Paul A. Maggard earned his Ph.D. in solid-state materials chemistry at Iowa State University in Ames, Iowa. Following a post-doctoral stint at Northwestern University in Evanston, IL, he accepted a faculty position in the Department of Chemistry at North Carolina State University. Current research efforts in his laboratory focus on the flux and hydrothermal mediated syntheses of crystalline metal oxides, carbon nitrides, and metal-oxide/organic hybrids and characterization and development of their photoelectrochemical properties for solar energy conversion. He currently holds the position of Professor and has published >100 papers and book chapters and has received several awards for his research, including the NSF CAREER award, Beckman Young Investigator award and a Scialog award for solar energy research.