



CHEMISTRY SEMINAR 291

Chemistry of Clean Energy Materials: From Halide Perovskites to Binary Metal Phosphides

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ABSTRACT

Our group is interested in the soft synthesis and chemical spectroscopy of optical nanomaterials. This talk will highlight some of our recent work in two areas:

Halide Perovskites: New Semiconductors for Energy Conversion. Halide perovskites are one of the most interesting semiconductors for photovoltaics, with solar cells made of these materials approaching power conversion efficiencies of 25%. We were among the first to synthesize colloidal $APbX_3$ ($A = \text{methylammonium}$; $X = \text{I, Br}$) nanocrystals, and showed that, at the single particle level, they display shape-correlated PL emission across whole particles, with little photobleaching and very few off periods [1-3]. In addition, we introduced solid state NMR to probe the extent of alloying and phase segregation in mixed ion halide perovskites [4-5], which show superior performance and stability. Because ^{207}Pb chemical shifts are highly sensitive to local coordination, electronic structure, and vary linearly with halogen electronegativity and band gap, ^{207}Pb ssNMR gives the true chemical speciation of samples made by different methods. Nonstoichiometric dopants and amorphous phases are prevalent in samples made from solution, while a novel solid phase synthesis, starting from the parent, single-halide perovskites suppresses phase segregation [6-7]. Our observations are consistent with the presence of miscibility gaps and spontaneous spinodal decomposition in these materials at room temperature, underscoring how different synthetic procedures impact their composition, nanostructuring, and properties. **Binary Metal Phosphides: From Hydrogen Evolution to Nitrate Removal from Water.** A better understanding of the chemistry of molecular precursors is useful in achieving more predictable and reproducible nanocrystal preparations [7-8]. Using commercially available organophosphite precursors, we have used a chemical reactivity approach to synthesize nickel and nickel phosphide nanocrystals with high selectivity (Ni , Ni_2P and Ni_3P_2 phases) [9]. Some organophosphites, such as $\text{P}(\text{OMe})_3$ or $\text{P}(\text{OiPr})_3$ transiently form zerovalent, metallic nickel; the latter is persistent with the bulky organophosphite $\text{P}(\text{O}-2,4\text{-tBu}_2\text{C}_6\text{H}_4)_3$. Along with other first row, transition metal phosphides, Ni_2P is a very active catalyst for the hydrogen evolution reaction, as well as for hydrodesulfurization, and other reforming reactions. Based on this information, we hypothesized that Ni_2P should be active in the reduction of oxyanions. Indeed, we have recently succeeded in using this material as a catalyst for the near ambient removal of nitrate from water.

BIO:

Dr. Javier Vela is an associate professor of chemistry at Iowa State University in Ames, Iowa, USA. He obtained his Lic. degree with Honors from UNAM in 2001, and M.S. and Ph.D. degrees from the University of Rochester in 2003 and 2005, respectively. He was a postdoctoral researcher at the University of Chicago from 2005 to 2006, and a Director's Postdoctoral Fellow at Los Alamos National Laboratory's Center for Integrated Nanotechnologies from 2007 to 2009. Dr. Vela's research focuses on low dimensional optical materials for energy, catalysis, and imaging applications. He is a member of the editorial boards of ACS Energy Letters and Wiley's ChemNanoMat. He has been named Fellow of the AAAS (2018), IUPAC Young Observer (2017), and received the NSF CAREER Award (2013).

