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AUSTIN, TEXAS

Will present a seminar on

“CORRELATING STRUCTURE AND FUNCTION FOR NANOPARTICLE CATALYSIS”

Metal nanoparticles of only ~100-200 atoms are synthesized using a dendrimer encapsulation technique to facilitate a direct comparison with density functional theory (DFT) calculations in terms of both structure and catalytic function. Structural characterization is done using electron microscopy, x-ray scattering, and electrochemical methods. Combining these tools with DFT calculations is found to improve the quality of the structural models. DFT is also successfully used to predict trends between structure and composition of the nanoparticles and their catalytic function for reactions including the reduction of oxygen and the oxidation of formic acid. This investigation demonstrates some remarkable properties of the nanoparticles, including facile structural rearrangements and nanoscale tuning parameters which can be used to optimize catalytic rates.

THURSDAY, OCTOBER 30, 2014
COOKIES AND COFFEE -- 1:45 P.M.
SEMINAR -- 2:00 P.M.
SARKEYS ENERGY CENTER, ROOM M-204

THIS IS A REQUIRED SEMINAR FOR CHE 5971

Accommodations on the basis of disability are available by contacting the office.