

Guerro's research focuses on catalytic nanostructured materials, mostly metal and oxide nanoparticles, to understand the relationship between catalytic performance and materials properties for applications such as hydrogen production and purification, CO oxidation, and greenhouse gas elimination. "I can hardly imagine my life outside science. I have been lucky. But what I have accomplished in the result of hard work, honesty, and true commitment to my work and my students. Troubles are always there. What is important is to put passion in your work, no matter what is your gender." While taking questions, Guerro also noted that young women are being involved more and more in scientific careers, likely due to the successful diffusion of knowledge to encourage young people to pursue scientific careers. She noted that challenges facing the Mexican female scientist include male-dominated evaluation committees and difficulties associated with publication when all authors have Latin surnames. Guerro was drawn to chemistry because, although she had "a lousy chemistry" teacher at a young age, the field continued to intrigue her and her cousin (who is a chemist) encouraged her studies.

TALKS

Symposium 1. Nanostructured Materials and Nanotechnology

Nanoparticle Synthesis and Assembly from Atomistic Simulation Studies

Nanoparticles are involved in 75% of today's chemical manufacturing processes (tires, toners, food, pharmaceuticals, waste, cosmetics, etc.), and controlled synthesis of these nanoparticles is critical for commercial success. Nanoparticles can be synthesized in a liquid phase, allowing for good control of particle size control but low production rate, or in a vapor phase, allowing for high productivity rates but has significant difficulties in controlling particle size. T. Hawa (University of Oklahoma) investigates synthesis variables on the effects of final nanoparticle physical properties by molecular dynamics simulations.

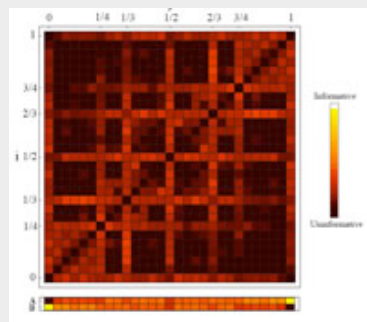
Vapor synthesis begins with a chemical precursor vapor that eventually breaks down and nucleates nanoparticles on a substrate. Final particle size is a balance particle-particle interactions: coalescence, where two particles combine to form one larger particle; and collision, where two particles collide to form one agglomerate. Hydrogen passivation is a common technique to tie up dangling bonds on the surface of nanoparticles and thus reduce their reactivity, and Hawa seeks to understand the effects of passivation on the balance of coalescence and collision during particle synthesis. Particle interaction is proportional to the contact surface area, and this data can be extrapolated to approximate the critical approach energy for the reaction. If the particle energy is lower than the critical reaction energy, then the particles will not react; if the energy is higher, then they will. Hawa also found that increasing particle temperature and decreasing particle size increases the probability of particle reaction. An equation for the coalescence time was obtained, and Hawa finds that hydrogen stays on the surface of the particle throughout coalescence. Effects of hydrogen passivation on the dynamics of sintering of individual particles and particle aggregates, as well as the stability of nanoparticles facets (from which the final particle shape can be predicted) were also investigated and compared to experimental results in the literature.

Nanoparticle assembly is one of the largest challenges in nanotechnology-based device development, and Hawa investigated electrostatic-directed assembly, both experimentally and by modeling. Electrostatic-directed assembly, where substrates have charged patterns that attract oppositely-charged particles, is a common and robust assembly technique. Hawa employed a GaAs substrate with regions of Si- and Zn-doping which formed p-n junctions. When a voltage was applied across the junction, charged particles were observed to collect on oppositely-charged regions of the substrate. Particle trajectory over like-charged substrate regions was modeled to determine the effect of the electric field to control particle deposition location.



Symposium 2. Theory and Computer Simulation of Materials

The Prediction of Crystal Structure by Combining Machine Learning Knowledge Methods with First Principle Energy Methods



Novel chemistry can result in crystal structures that we can't currently predict-- "This is a serious problem," comments Gerbrand Ceder (Massachusetts Inst. Tech.). Crystal structures are difficult to predict because there are many possible structures competing for dominance, in addition to an inherently complicated energy landscape. Current prediction techniques find the ground-state crystal structure by beginning with an energy model and then directly optimizing the coordinates to select the system with the minimal ground state energy; yet, physics is only used in the initial energy model, whereas injecting physics into the energy landscape can allow smarter searching through statistical learning. Ceder employs structure assignments from large experimental databases to "learn" the underlying physical rules that governs crystal structures, and then captures this knowledge in a mathematical model by building a probability density for structures to coexist in a chemical system-- in other words, systems with the same underlying physics. Finally, he uses this knowledge-optimized model to predict crystal structures through density functional theory (DFT), which he showed to be accurate in predicting crystal structures ~97% of the time for 80 binary systems.

Ceder used his mathematical model to compute a candidate list for the crystal structure of AgMg_3 which is known as a compound with an unknown structure. Cu3P-type structure, an uncommon structure that occurs only five times in all binary