LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

Spring Seminar Series
3:30pm - 4:30pm, Wednesday February 20, 2013
Johnston Hall 338, Louisiana State University

Deliberate Discovery of Missing Materials and the "Inverse Problem": Given a Desired, Target Property, Find the Structure

by

Prof. Alex Zunger

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Condensed matter physics and material research has historically often proceeded via trial-and-error or even accidental discoveries of materials with interesting physical properties, including new ferromagnets, superconductors, magneto–resistors, transparent-conductors, carbon nanotubes, etc., etc. The question posed in this talk is: does it make sense instead to first declare the physical property you really want, then find which structure/material has this property? I will describe recent advances in the way quantum-mechanical electronic structure calculations have been combined with biologically-inspired ("genetic") evolutionary approaches to scan a truly astronomic number of atomic configurations in search of the one that have desired, target electronic properties ("Material Genome Initiative"). Recent examples of such "*Inverse Design"* in the areas of nanostructures, magnetism, semiconductors and spectroscopy will be mentioned. This work was also borne out of the recognition that many materials that can be expected to exist, are in fact missing from the compilations of all materials previously made. Are they missing for a good reason (i.e., they are intrinsically unstable), or did people did not get around to making them yet, but they could have interesting properties? I will describe the way modern "first principles thermodynamics" can address this question, and in the process discover quite a few inorganic structures and materials that *should* exist, but are yet undiscovered. Experimental efforts to make such materials are underway in the newly formed "Energy Frontier Research Center on Inverse Design."

Prof. Alex Zunger research field is "Theory of Real Materials", and a pioneer in the field now called "First Principles Theory of Solids". He has applied this technique in the past ~30 years to a broad range of materials classes (semiconductors, insulators, metals, molecular crystals), geometries (nanostructures, surfaces, interfaces, alloys), and properties (spectroscopic, thermodynamic, structural). This work has been recognized by some of the leading awards in physics including the year 2012 (inaugural) *"Material Theory Award" of the MRS*; the *John Bardeen award of The TMS*, the *Rahman Award of the American Physical Society*, the *Gutenberg Award* for science (Germany), as well as the upcoming (year 2013) *Hume-Rothery Award* on theory of alloys. He mentored 77 postdoctoral fellows, published over 600 papers in refereed journals, including over 150 in Physical Review Letters and Rapid Communication. His papers have received over 50,000 citations, and his high "*h-index"* is over 100 (100 of his papers were cited each at least 100 times). He is the author of the fifth-most-cited paper in the 110-year history of Physical Review (out of over 350,000 articles published in that journal). He pioneered the science of materials by design now used in the "Materials Genome Initiative" (MGI) established the "Energy Frontier Research Center on Inverse Design" – a USA Office of Science Center involving more than 40 researchers. He is its Chief Scientist, working at the University of Colorado, Boulder.

This seminar will be broadcast at the following venues: Liberal Arts Building 234 (UNO), Qatar Pavilion Conference Room 226 (Xavier University), JB Moore Hall Room 211 (Southern University), PML 1015, Center for Instructional Technology, at the Wyly Tower (LA Tech), and via Adobe Connect at https://connect.lsu.edu/la-sigma/ .