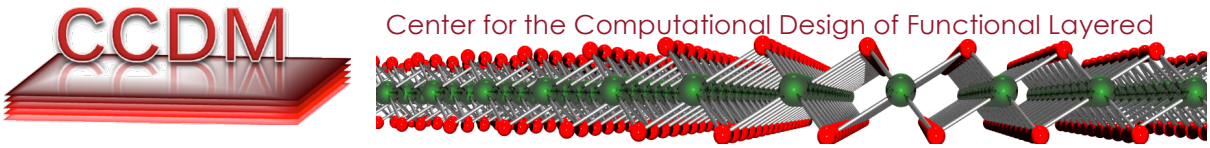

May 12, 2017
Temple University, SERC Room 703, 12:30 PM

New Functional Materials as a Design Problem

Alex Zunger, *University of Colorado, Boulder, CO*
http://www.colorado.edu/zunger-materials-by-design

The history of material research and condensed matter physics has often proceeded via accidental discovery of compositions and structures with interesting physical properties – superconductors, Photo catalytic compounds, magneto-resistors to name a few. Yet, for many applications we know well what type of physical properties we want, except that we do not know a material that has those target properties. The question posed in this talk is: does it make sense to first declare the property you really want, then find the structure and material that has this property. The obvious obstacle is that there are innumerably many possible atomic structures that could, in principle, be made even from a few elements and we do not know which structure would have the desired target property. It turns out that modern atomic-resolution quantum mechanics (i.e., electronic structure theory) can be combined with biologically- inspired (evolutionary) " Genetic Algorithms" to scan a truly astronomic number of atomic configurations in genomic-like search of the one(s) that have desired, target materials properties. Once the number of configurations with target property is narrowed down to a few, laboratory synthesis becomes viable. Once narrowed down, conventional growth, optimization etc takes place. Some examples of crystalline materials will be given where unexpected discoveries were possible.

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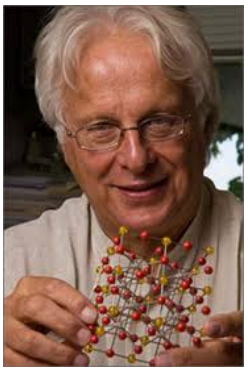

Prof. **Alex Zunger** of the University of Colorado, Boulder research field is *Condensed Matter Theory of Real Materials*, involving foundational work on Density Functional Theory, total energy and force formalism, and first first principles Pseudopotentials . He received his degrees at the Tel Aviv University, Israel with post docs at Northwestern and U.C. Berkley. He is the recipient of the year 2013 **Hume- Rothery Award** on Theory of alloys, the 2011 (inaugural) **"Materials Theory Award"** of the Materials Research Society on Inverse Design, the 2001 **John Bardeen award** of The Material Society on "Spontaneous Ordering in semiconductor alloys", the 2001 **Rahman Award** of the American Physical Society on 'foundational development of First Principles methods', the 2010 "**Tomassoni Prize"** (Italy) and "**2010 Medal of the Schola Physica Romana** " celebrating the tradition of E. Fermi, and the 2009 **Gutenberg Award** (Germany) on correlated electron systems. He is a Fellow of the American Physical Society; Fellow of the Materials Research Society, Sakler Fellow of the Institute of advanced studies of Tel Aviv University. He has been the founding Director of the $20 million 'Center for Inverse Design' (a DOE Energy Frontier Research Center). The impact of Dr. Zunger's work is partially reflected by the very high number of citations his papers have received (over 80,000, according to Google Scholar) and by his "h-number" of 130 .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.