Abstract for an Invited Paper
for the MAR07 Meeting of
The American Physical Society

Quantum-Mechanical Combinatorial Design of Solids having Target Properties[1]

ALEX ZUNGER[2], National Renewable Energy Laboratory, Golden, Colorado 80401

(1) One of the most striking aspects of solid state physics is the diversity of structural forms in which crystals appear in Nature. Not only are there many distinct crystal-types, but combinations of two or more crystalline materials (alloys) give rise to various local geometric atomic patters. The already rich repertoire of such forms has recently been significantly enhanced by the advent of artificial crystal growth techniques (MBE, STM- atom positioning, etc.) that can create desired structural forms, such as superlattices and impurity clusters even in defiance of the rules of equilibrium thermodynamics. (2) At the same time, the fields of chemistry of nanostructures and physics of structural phase-transitions have long revealed that different atomic configurations generally lead to different physical properties even without altering the chemical makeup. While the most widely - known illustration of such "form controls function" rule is the dramatically different color, conductivity and hardness of the allotropical forms of pure carbon (diamond,graphite, C60), the physics of semiconductor superstructures and nanostructures is full of striking examples of how optical, magnetic and transport properties depend sensitively on atomic configuration. (3) Yet, the history of material research has generally occurred via accidental discoveries of material structures having interesting physical property (semiconductivity, ferromagnetism; superconductivity etc.). This begs the question: can this discovery process be inverted, i.e. can we first articulate a desired target physical property, then search (within a class) for the configuration that has this property? (4) The number of potentially interesting atomic configurations exhibits a combinatorial explosion, so even fast synthesis or fast computations can not survey all. (5) This talk describes the recent steps made by solid state theory + computational physics to address this "Inverse Design" (Franceschetti & Zunger, Nature, 402, 60 (1999) problem. I will show how Genetic Algorithms, in combination with efficient ("Order N") solutions to the Pseudopotential Schrodinger equation allow us to investigate astronomical spaces of atomic configurations in search of the structure with a target physical property. Only a small fraction of all ($\sim$ 10**14 in our case) configurations need to be examined. Physical properties are either calculated on-the-fly (if it's easy), or first "Cluster-Expanded" (if the theory is difficult). I will illustrate this Inverse Band Structure approach for (a) Design of required band-gaps in semiconductor superlattices; (b) architecture of impurity –clusters with desired optical properties (PRL 97, 046401, 2006) (c) search for configuration of magnetic ions in semiconductors that maximize the ferromagnetic Curie temperature (PRL, 97, 047202, 2006).

[1]Supported by DOE-SC-BES-DMS and DARPA under NREL DEAC36-98-GO10337.
[2]In collaboration with S. Dudiy, A. Franceschetti, W. Jones and K. Kim.