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Quantum-Mechanical Combinatorial Design of Solids with Target Properties¹

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One of the most striking aspects of solid-state physics is the diversity of structural forms in which crystals appear in Nature. The already rich repertoire of such (equilibrium) forms has recently been significantly enriched by the advent of artificial growth techniques (MBE, STM- atom positioning, etc) that can create desired structural forms, such as superlattices and geometric atomic clusters even in defiance of the rules of equilibrium thermodynamics. As is well known, different atomic configurations generally lead to different physical properties even at fixed chemical composition. While the most widely-known illustration of such “form controls function” rule is the dramatically different color, conductivity and hardness of the allotropic forms of pure carbon, the physics of semiconductor superstructures and nanostructures is full of striking examples of how optical, magnetic and transport properties depend sensitively on atomic configuration (e.g, compare the properties of random to ordered alloys). Yet, the history of material research generally proceeded via accidental discoveries of materials configuration with interesting physical property (semiconductivity, ferromagnetism; superconductivity etc). Given the ability of growing many different atomic configurations, and given the often sensitive dependence of physical properties on atomic configuration, makes one wonder: can one first articulate the desired target physical property, then search (within a class) for the configuration that has this property? This talk describes the recent steps made by solid-state theory and computational physics to address this “Inverse Design” problem. I will show how Genetic Algorithms, in combination with efficient (“Order N”) solutions to the Pseudopotential Schrödinger equation allow us to investigate astronomical spaces of atomic configurations in search of the structure with a target physical problem. Only a small fraction of all ($\sim 10^{14}$ in our case) configurations need to be examined. Examples will include Band-Gap design in superlattices; architecture of impurity-clusters with desired optical properties, and Inverse Design of the Curie temperature in dilute magnetic systems.

¹This work was performed in collaboration with A. Franceschetti, P. Piquini, S. Duidy.