INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

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Designing Materials by Combining *Ab Initio* Methods and Optimization Algorithms

In this seminar, I will describe the application of first-principles methods and optimization algorithms to accelerate the discovery of new materials. First, I will address the problem of searching for new *p*-type, i.e., hole-conducting, transparent compounds. I will then turn to the problem of predicting the crystal structure of materials starting from the chemical composition.

Optimum *p*-type transparent conducting materials must satisfy several design criteria: (a) possess a large concentration of hole-producing defects, (b) have high hole conductivity, and (c) have an optical absorption edge above the transparency threshold. We selected the Cu3VO4 and Ag3VO4 oxovanadates from a pool of candidate noble-metal oxides and applied *ab initio* methods, based on density functional theory, to assess whether they meet the above design criteria. We predicted that Ag3VO4 (i) is a *p*-type material with a hole concentration of ~1014 cm-3 at room temperature along with a very low concentration of hole-killing defects, (ii) has a hole effective mass lower than that of the prototypical *p*-type transparent conducting oxide, CuAlO2, and (iii) is on the verge of transparency (i.e., transparent to red light).

Crystal structure prediction, given only the elemental components of a solid and without constraints on the lattice vectors and atom positions, is a central problem in solid state physics. Solving this problem requires a global space-group optimization (GSGO) of the total energy of a solid as a function of the crystal degrees of freedom. Evolutionary algorithms are powerful global optimization methods, and I will describe a procedure based on an evolutionary algorithm to address the GSGO problem. First, I will illustrate an application of the GSGO method to selected binary systems with fixed compositions, including Cd-Pt, Al-Sc and Pd-Ti. I will then extend the GSGO algorithm to predict the compositions, as well as the crystal structures, of the thermodynamically stable phases of a solid system, and will present an application of this variable-composition GSGO method to the Al-Sc alloy.