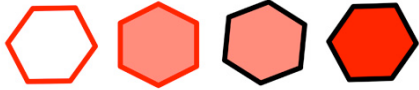


MARVEL



NATIONAL CENTRE OF COMPETENCE IN RESEARCH
MATERIALS' REVOLUTION: COMPUTATIONAL DESIGN
AND DISCOVERY OF NOVEL MATERIALS



ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

NCCR MARVEL Distinguished Lecture

The Inverse Problem in materials theory: Find the system that has a given target property

Prof. Alex Zunger

University of Colorado, Boulder, Colorado

Thursday 9th October, 16:15, Room MXF-1

The history of material research and condensed matter physics has often proceeded via accidental discovery of materials with interesting physical properties – superconductors, solar absorbers, light-emitting semiconductor, 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 innumerable 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 now 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. I will describe recent progress in this exciting endeavor of “Inverse Design”. **Examples will include nanostructures by design, impurity-physics by design, magnetism by design, and the discovery of hitherto missed, new inorganic crystals.**