The Inverse Problem in Nano science and in materials theory: find the system that has desired target properties

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The history of material research generally proceeded via accidental discoveries of materials configuration with interesting physical property (semiconductivity, ferromagnetism; superconductivity, etc.). The question posed in this talk is: Given that structure /configuration often decides the material's property, and given that many (in fact, an astronomic number of) possible structures can be made, does it make sense to first declare the material property you really want, then find that structure and material that has this ?

This talk will focus on the way atomistic electronic structure calculations are combined with evolutionary algorithms to scan a truly astronomic number of atomic configurations in search of the one(s) that have desired, target electronic properties. Thus, instead of using atomic structure (configuration) as input and electronic properties as output, we will do the reverse: use electronic properties as input and obtain configuration as output.

This work was also borne out of the recognition that many inorganic materials that can be expected to exist, are in fact missing from the compilations of materials that were ever made. Are they missing for a good reason (i.e, are intrinsically unstable) ,or are they missing for no good reason (people did not get around to make them yet) .I will describe a format of first-principles calculations that can address this question, and in the process discover quite a few inorganic structures (e.g, oxides) that should exist, but were yet undiscovered.

Current examples of Inverse Design include (i*) Design of nanostructure* band gap (e.g which superlattice sequence of GaAs/AlAs will have a given value of band gap ? Can one find a sequence of Si/Ge/Si… that has a truley direct and optically strong gap ?) (ii*) Impurity by design* (e.g which arrangement of nitrogen impurities in GaP will have the deepest, or the shallowest impurity level ?) (iii*) Ferromagnetism by design* (e.g, can one find a structure of Mn in GaAs with a given Curie temperature ?) (iv) *Excitonic spectra by design* (e.g, can one find a structure of a quantum dot that has a given sequence—barcode—of excitonic lines ?) .(v) Search of transparent conductors (e, g, look for those structures that would have high hole conductivity).