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

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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 innumerably 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**.