Understanding-based discovery of Functional Materials: The Inverse Design Paradigm

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In the last half century, our understanding of electronic, magnetic and structural properties of matter has been transformed from text-book 'Model Hamiltonian' description of schematic cartoons of solids to a predictive theory Real Materials. This has opened the door for laboratory experiments trying to replace accidental discovery of functional materials by understanding-based search-and-design of materials with given target properties. The present talk will discuss the origins of such Inverse Design paradigm of rational discovery of functional materials and the important role of the concomitant surge of data bases of computed material property and their use in machine learning.