

From Metaheuristic to dynamical crystal structural search from first principles

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In recent years, computational materials science has been recognized for its materials prediction proficiency as well as the possibility of working together with experiments with a common goal: *materials design*. The prediction of low energy crystal structures only based on the knowledge of its chemical composition is complex NP optimization problem. Independently of the methodology used to describe the atomic interactions, which can go from parameterized classical potentials to the quantum nature of the electrons and ions, it is possible to develop methods that can search efficiently over the Born Oppenheimer surface, avoiding largely the exponentially complexity with respect to the number of atoms. This problem has been recognized within the "Materials Genome Project", where synergistic approaches from theory and experiment have proven to be very successful in addressing the materials design problem. In this direction, I will describe our efforts in creating a flexible computational package that, by using a large set of methods, will search over potential crystal structures (stable and metastable) based uniquely on the chemical composition. I will demonstrate its use by presenting different applications ranging from lead based thermoelectrics, lithium batteries to crystal topological materials.