THEORETICAL AND COMPUTATIONAL MODELING OF MULTI-ANION CHEMICAL SYSTEMS: AN EVOLUTIONARY APPROACH

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In the talk, I will discuss the materials modeling approach that we use in our group to describe many unique properties on the atomic scale. This approach is an evolutionary strategy that connects and combines the crystal-chemical modeling, a combination of experimental data, theoretical methods, and computational algorithms. In particular, three different key tools - lattice geometry along with group theory considerations (periodic structure generation), quantum chemistry arguments (the concept of long- and short-range interactions) and relevant DFT simulations (the discrete optimization framework) - are combined together to provide an overall view of composition-structure-function relationships at various levels of complexity. This model opens the way for the prediction of a wide range of new stable compounds with different 2D and 3D crystal architectures.

Our research was motivated by the experimental work made on the synthesis and understanding of the various properties of multi-anion chemical systems [1,2]. Multi-anion compounds that contain two or more kinds of anions are known as metal oxyfluorides, oxychlorides, oxyhydroxides and oxyhydrides. They exhibit a number of interesting properties which can be used in the design and development of new functional materials [3,4]. However, the study of these systems has raised a number of fundamental questions concerning the key factors and basic mechanisms responsible for the formation as well as the structural and electronic features of these materials. In the context of multifunctional properties, I will characterize the technological perspective related to the various possibilities of application of these materials.

References

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