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Informatics guided computation of physical and chemical properties of nanomaterials

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The aim of this presentation is to describe how we use informatics to first identify key electronic and crystal structure, and use that information to guide fundamental electronic structure of materials to explore their reactivity. Particular focus will be directed towards the use of density of states, band structure, charge density and electron localization functions. Informatics is an emerging field in the discovery and development of new materials. The different techniques used are deployed to scour large databases in order to find novel and useful patterns that might otherwise remain unknown, converting raw data into useful information. Thus, in material sciences, it can provide important information about what parameter (element, site, among others) it is important to improve a specific property in a material. Our research platform is based on the study materials in the family of apatite structure types, both of which have the ability to accommodate numerous chemical substitutions. Both these classes of materials exhibit a broad range of multifunctional properties and have demonstrated an even newer array of properties when in a nanostructure form. The rich chemistry and structural diversity of apatite provides fertile ground for the synthesis of technological relevant compounds. By mean of computational calculations (quantum and classical mechanics) we can obtain structural, dynamical, thermodynamic, electrical, among others properties for bulk and surface of apatite. In this work we will present the electronic structure and bonding properties of a group of, knows and provided by Informatics, fluorapatites by mean of *ab initio* calculations.

Biography

Claudia Loyola Canales has obtained the Undergraduate Physics degree in the Facultad de Ciencias, at Universidad de Chile in 2005 and the PhD in Physics in 2010. The PhD thesis was conducted by Professor Gonzalo Gutiérrez. Later, she spent three years at the COSMIC Group at Iowa State University in USA as a Postdoctoral Research Associate supported by the Postdoctoral Fellowship Becas Chile. She returned to Chile, and join to the Physics Department at Universidad Andrés Bello as an Assistant Professor in January 2015. She has published nine papers in reputed ISI journals up today.

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