

Physics Colloquium

Michigan Technological University

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Room 139, Fisher Hall

Ab initio Properties of Materials

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Abstract

Periodic boundary conditions are widely adopted in solid-state physics and materials science to model systems with perfect crystalline structure or localized defects. The *ab initio* quantum-mechanical CRYSTAL code is one of the tools available for the calculation of the electronic structure and properties of crystals. It is based on a description of the electronic wave function in terms of linear combinations of atomic orbitals (LCAO), which permits an easy interpretation of the electronic structure and a direct comparison with molecular fragments.

A large variety of properties of matter in the condensed phase can be calculated with the present release of the code, CRYSTAL03. The performance of the CRYSTAL code will be illustrated through a few examples: the structural properties of katoite (hydrogarnet), a possible candidate for hydrogen storage; the study of ferro- and anti-ferro-magnetic phases of a series of transition metal fluorides with perovskite structure and analysis of the super-exchange interaction; dielectric properties of materials.



Roberto Orlando's research activity is in the field of Theoretical Chemistry of condensed phases, both concerning the implementation of the methods and their application to the solution of problems in materials science, geochemistry, surface science and catalysis. The main product of this research is a quantum mechanical *ab initio* computer code, CRYSTAL, which was released to the scientific community first in 1988 and of which he is a co-author.