BENEMÉRITA UNIVERSIDAD AUTÓNOMA DE PUEBLA

INSTITUTO DE FÍSICA
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SEMINARIO EXTRAORDINARIO
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"Crystal structures prediction using ab initio evolutionary algorithm USPEX and DFT calculations."

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The prediction of crystal structure from the unique knowledge of its chemical composition has been a long-standing challenge in materials science. Indeed, this goal is far from trivial: how to reach the global minimum as fast as possible among the millions of potentially existing crystal structures for a system containing only 10 atoms per cell (1)? An effective and robust code, USPEX (2), attempts to address this problem. It is based on an evolutionary algorithm (EA) which mimics Darwinian evolution and employs natural selection of the fittest and such variation operators as genetic heredity and mutations. The EA developed by A.R. Oganov et al enables reliable prediction of the stable crystal structure without relying on any experimental data. USPEX has resulted in a number of predictions of hitherto unknown stable structures and is an extremely valuable tool in computational materials discovery (3). I will give a short overview of the USPEX method and I will highlight this powerful approach in determining the crystal structure of materials by recent findings coming from the USPEX community (3). Thereafter, I will focus on our on-going researches in my group (4), looking at the chemical bonding in predicted crystals by the help of molecular orbital (MO) analysis and other chemist's tools: a- does MoN2 have the experimentally claimed layered MoS2-like structure? b- cyclic H3)+ cations stabilized in high-pressure H3Cl phase: emergence of unusual stoichiometries in solid state chemistry."

(1) The number of distinct points on the energy landscape is roughly 10^N, with N is the number of atoms in a unit cell.
(2) USPEX :
http://uspex.stonybrook.edu/uspex.html>http://uspex.stonybrook.edu/uspex.html;
(3)http://uspex.stonybrook.edu/uspexpublications.html>http://uspex.stonybrook.edu/uspexpublications.html; http://dnnsm2015.conference.univ-poitiers.fr
(4) (a) Hu C.-H., Frapper G., et al (2013) "Pressure-Induced Stabilization and Insulator-Superconductor Transition of BH ". Phys. Rev. Lett.; (b) Yu S., Frapper G. et al (2014) "Exploration of stable compounds, crystal structures, and superconductivity in the Be-H system" AIP Advances; (c) ibid (2015) "Pressure-driven formation and stabilization of superconductive chromium hydrides", Scientific Reports; (d) ibid (2015) "Phase stability, chemical bonding and mechanical properties of titanium nitrides: a first-principles study", PCCP; (e) ibid (2016) "Exploring the Real Ground-State Structures of Molybdenum Dinitride " submitted to JPC C, march 2016.

Auditorio-IFUAP
Viernes 15 de Abril de 2016
18:00 Hrs.