ST. FRANCIS XAVIER UNIVERSITY

Department of Mathematics, Statistics and Computer Science

St. Francis Xavier University

Presents

Searching for New Materials for the Hydrogen Car: Computational Challenges

by

Dr. Iván Cabria

Department of Theoretical Physics

University of Valladolid, Spain

Monday, Oct 22nd, 2012 @ 2:15 AX23A

Hydrogen storage is the bottleneck of the present hydrogen car technology. Scientists are looking for light and porous materials that store enough hydrogen on-board to obtain a hydrogen car with the same autonomy as a gasoline car, about 600 km. Computational simulations of new materials are used to predict and/or explain their hydrogen storage capacities. Those simulations consist on solving the Density Functional Theory (DFT) equations and/or Molecular Dynamics (MD) of the materials. Computer Science methods are useful to improve the speed of the MD simulations. This talk will explain the hydrogen car, the hydrogen storage technological goals, the different materials studied for hydrogen storage on experiments and simulations and the parallel MD simulations. Then, we will show a Mean Shift-Based initialization method for K-means that increases the speed of parallel MD simulations and can also be applied to another fields.

Refreshments will be served before the talk in AX24A