The Department of Mathematics, Statistics and Computer Science

St. Francis Xavier University

presents

Monte Carlo and Molecular Dynamics Simulations of Hydrogen Storage on Carbon Nanopores

by

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Monte Carlo, MC, and Molecular Dynamics, MD, are computational methods used to explain the properties of materials and to improve the design of new materials. They are computationally demanding and therefore, many research efforts are devoted to improve their algorithms. The main algorithms, serial and parallel, used in MC and MD will be explained. Applications of MC and MD to the study of the hydrogen storage capacities of carbon nanopores will be also presented and explained. These materials are promising candidates to store enough hydrogen for automotive applications.