ST. FRANCIS XAVIER UNIVERSITY

Physics Colloquium

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Friday, 9 October 2009
4:00pm, PSC 3046

Molecular simulations: from kidney stones to perpetual motion machines

In this talk, I will discuss how computational modelling starting from basic physical principles can be used to gain a better understanding of biological processes and phenomena at the atomic level. I will briefly overview the library of computational approaches [1] and then demonstrate how simulations and modelling can used to understand cellular membranes and their interactions with biologically important molecules, the formation of kidney stones and other biologically important phenomena. I will also address the question of how simulations can be compared with experiments, and how simulations can provide experimentally testable predictions. Finally, I will discuss some of the problems and subtleties related to simulations; apparent perpetual motion being one of them.

1. Multiscale modeling of emergent materials: biological and soft matter
T. Murtola, A. Bunker, I. Vattulainen, M. Deserno, and M. Karttunen
PCCP 11, 1869-1892 (2009).

For further information on Physics colloquia visit http://physics.stfx.ca
Doughnuts and coffee will be served at 3:45 pm