



The PHYSICS DEPARTMENT

invites you to attend a seminar by:



DR. OLEG RUBEL

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Adjunct Professor, Department of Physics
Lakehead University

“Band structure of disordered solids: from localization to high-mobility Kane fermions”

Supercells are often used in *ab initio* calculation in order to model compound alloys, surfaces and defects. One of the main challenges of supercell electronic structure calculations is to recover Bloch character of electronic eigenstates perturbed by a disorder. Here we apply the spectral weight approach to unfolding of the electronic structure of group III-V and II-VI semiconductor solid solutions. The illustrative examples include: formation of localized donor-like states in dilute GaP:N and associated enhancement of its optical activity, direct observation of the valence band anticrossing in dilute GaAs:Bi, and a topological band crossover in ternary (HgCd)Te alloy accompanied by emergence of high-mobility Kane fermions. The analysis facilitates interpretation of optical and transport characteristics of alloys that are otherwise "obscure" in traditional first-principle supercell calculations.

DATE: Wednesday, MAY 21st, 2014

TIME: 10:00 am

Room: CB 4058