# Materials Science and Technology Division

## "Modeling Charge Transfer of Defects in ceramics and nonlinearity in detector materials"

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Thursday, May 6, 2010
11:00 a.m.
HTML/ 4515, Room 265

**Abstract:**

The effects of charge transfer on defects and defect generation in ion-solid interactions in ceramics are being modeled at the atomic scale, and multiscale models are being applied to the study of nonlinearity in detector materials. —Large-scale *ab initio* simulation methods (up to a few thousand atoms) have been developed for the study of ion-solid interactions in materials, and they are employed to investigate the primary damage states for primary knock-on atom (PKA) energies up to 1 keV in SiC and GaN. These simulation results provide important insights into electronic effects on ion-solid interaction processes, revealing that significant charge-transfer occurs between recoiling atoms. The charge variation of the PKA can decrease the energy barrier for stable defect formation, and the corresponding dynamic evolution of a stable defect is a charge-assisted process, which is expected to have significant effects on defect creation in covalent and ionic materials. Thousand-atom *ab initio* simulations provide a feasible path for studying low-energy ion-solid interactions, charge transfer and charge-redistribution, with first-principle accuracy, in covalent materials.

In the second part of the presentation a multi-scale physics model developed at PNNL will be described, which consists of an advanced Monte Carlo method to simulate the production of electron-hole pairs and their nano-scale spatial distribution, as well as a kinetic Monte Carlo (KMC) model to study the efficiency of scintillation processes. Collectively, the theoretical results provide new insights into the processes involved in the information carrier yield, intrinsic variance, spatial distribution of electron-hole pairs, thermal transport of electrons and holes and the evaluation of possible mechanisms responsible for nonlinear (NL) effects in detector materials.

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