Virginia Tech Physics Department presents:

Prof. Shiwei Zhang (College of William and Mary)

"A Stochastic Field-theory Approach to Electronic Structure of Materials"

Abstract:

Understanding and predicting the properties of quantum many-particle systems remain an outstanding theoretical and computational challenge. In materials simulations, the standard model is an independent-electron approach in the framework of density-functional theory. In many materials where the effects of electron interaction are strong, this approach is inadequate. Several alternatives are being actively pursued. Among these, we have been developing a many-body, non-perturbative approach using auxiliary fields and stochastic sampling. Our approach takes the form of an ensemble of independent-electron calculations in fluctuating external fields. The different field configurations are "entangled" by random walks, and an approximate many-body wave function is obtained as a linear superposition of independent-electron solutions. I will discuss progress and prospects in the development and application of this approach. Results will be presented on electronic structure computations in atoms, molecules, and bulk materials.

Friday, Nov. 3

2:30 P.M.

210 Robeson