TSF16-2016-000101

Abstract for an Invited Paper
for the TSF16 Meeting of
the American Physical Society

Ab Initio Density Functional Studies of Nanoscale Materials[1]

IGOR VASILIEV, New Mexico State University

Nanomaterials exhibit a variety of unusual physical characteristics resulting from the interplay of quantum confinement and electronic correlations. The unique properties of nanomaterials make them attractive candidates for a broad range of applications in electronics, photonics, photovoltaics, chemistry, catalysis, and materials engineering. The properties of nanoscale structures can be tailored for specific applications by surface modification, chemical functionalization, and doping. My talk will focus on ab initio static and time-dependent density functional calculations for predicting the electronic, optical, magnetic, and transport characteristics of nanoscale materials. The flexibility of the density functional computational approach will be illustrated by its application to several different types of nanostructures, including doped and functionalized carbon nanotubes, graphene, surface-passivated semiconductor nanocrystals, and multiferroic perovskite thin films.

[1]Supported by NSF CHE-1112388