Multi-Paradigm Simulations at the Nanoscale: Methodology and Applications to Functional Carbon Materials

Haibin SU[1]
[1]*Division of Materials Science, Nanyang Technological University, Singapore*

Abstract

Multiparadigm methods to span the scales from quantum mechanics to practical issues of functional nanoassembly and nanofabrication are enabling first principles predictions to guide and complement the experimental developments by designing and optimizing computationally the materials compositions and structures to assemble nanoscale systems with the requisite properties. In this talk, we employ multi-paradigm approaches to investigate functional carbon materials with versatile character, including fullerene, carbon nanotube (CNT), graphene, and related hybrid structures, which have already created an enormous impact on next generation nano devices. The topics will cover the reaction dynamics of C60 dimerization and the more challenging complex formation dynamics in the nano carbon structures; the predicted magnetic state in NanoBuds; and opto-electronic properties of graphene nanoribbons.