Geometric and Energetic Aspects of SiC Nanostructures

Ming Yu
Department of Physics and Astronomy, University of Louisville, KY

Bulk SiC exhibits robust electrical, thermal, and mechanical properties. It possesses high strength, high thermal conductivity, stability at high temperature, high resistance to shocks, low thermal expansion, high refractive index, wide (tunable) bandgap and chemical inertness. Because of its outstanding physical properties, bulk SiC has now become one of the most promising materials for power electronics, heterogeneous catalyst supports, hard materials, and biomaterials. It is of interest, therefore, to understand how these properties would be modified in SiC nanostructures. Furthermore, bulk SiC manifests in many polymorphic forms due to different stacking arrangements of Si/C bilayers in cubic zinc-blended and the hexagonal wurtzite structures along the c-axis and the <0001> -direction, respectively. It is, therefore, natural to ask the question: "how such polymorphism will manifest itself in quasi-one and two-dimensional structures of SiC"? With this in mind, we have systematic investigated the structural stability of SiC nanostructure from energetic considerations, stacking arrangements, *etc*. employing quantum mechanics based simulation approaches. In this talk, I will present and discuss our the results including (i) the formation of the bucky-diamond structure of SiC clusters, (ii) the morphology, stability, and the electronic properties of SiC nanowires, and (iii) the energetic and electronic structures of graphitic-like and tubular Silicon Carbides.