Computational studies of Dirac fermion materials and nanostructures

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Graphene and topological insulators are among the most remarkable scientific discoveries of the past decade. High-performance computing plays important role in exploring various aspects of the physics of these novel materials and derived nanostructures. In my talk, I will cover our recent studies in the field of Dirac fermion materials which involve computational methods of various complexities: model Hamiltonian approaches applied to large nanostructures, density functional theory and many-body perturbation theory techniques. In particular, I will focus on the electronic properties of chiral graphene nanoribbons and on the electronic transport in polycrystalline graphene. Finally, I will discuss our recent investigations of the bismuth-based bulk topological insulators.