MAR10-2009-004272

Abstract for an Invited Paper
for the MAR10 Meeting of
the American Physical Society

Theory of charge transport in nanostructures: graphene and molecular junctions[1]

STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Laboratory

We discuss some recent progress on the theory and computation of charge transport in nanostructures. Selected results on two classes of systems of current interest – single molecule junctions and graphene nanostructures – are presented. Electronic level alignment at the metal-molecule contact (central to the conductance) is shown to be strongly renormalized by many-electron interaction (self-energy) effects. By including the environment-dependent quasiparticle self-energy correction to the molecular resonance levels, we obtain conductance values for amine-gold linked single-molecule junctions in good agreement with experiment, illustrating the importance of these many-electron effects in off-resonant conduction. The calculations also provide insights into the nature of the conducting molecular states and the influence of contact geometries. In graphene, the low-energy electronic states behave like two-dimensional massless Dirac fermions with pseudospin character. We show that this unique electronic structure leads to a number of novel properties in graphene and graphene-based nanostructures. Graphene nanoribbons are semiconductors with unusual electronic, magnetic and optical properties. The carrier dynamics in graphene exhibits anomalous anisotropy when subjected to an external periodic potential of nanometer dimensions (called graphene superlattices). Under appropriate conditions, these graphene superlattices are predicted to be electron supercollimators and new generations of massless Dirac fermions may be created. Charge transport across grain boundaries in graphene is also found to be highly unusual.

[1]This work was supported by NSF Grant No. DMR07-05941 and the U.S. DoE under Contract No. DE-AC02-05CH11231.