

Abstract Submitted  
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**First-principles Calculations of the Quasiparticle and Optical Excitations in Metallic Carbon Nanostructures**<sup>1</sup> JACK DESLIPPE, CHEOLHWAN PARK, MANISH JAIN, STEVEN LOUIE, UC Berkeley and Lawrence Berkeley National Lab — The band structure of metallic single-walled carbon nanotubes (SWNTs) may be viewed as a cut of the graphene band structure through the Dirac point. Despite the screening due to carriers at the Fermi energy, metallic nanotubes have been predicted theoretically and confirmed experimentally to exhibit strong many-electron interaction effects in their quasiparticle and optical properties, including the existence of excitons. We have carried out a systematic study, based on the first-principles GW approach, of the quasiparticle properties of metallic nanotubes with diameters ranging from 0.5 to 1.5 nm as well as those of single-layer graphene sheets. We present results (converged with a very fine k-point grid) using both the generalized plasmon-pole (GPP) model as well as a direct treatment of dynamic screening from the RPA dielectric response. We calculate the quasiparticle band structures, lifetimes and spectral functions for both the doped and undoped cases. We present first-principles calculations of excitons and the optical response of metallic carbon nanotubes for the same range of diameters within the Bethe-Salpeter approach.

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