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Band Gaps and Quasiparticle Energies of Graphene Nanoribbons¹ LI YANG, CHEOL HWAN PARK, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, YOUNG-WOO SON, School of Computational Sciences, Korea Institute for Advanced Study, Seoul 130-722, Korea, MARVIN L. COHEN, STEVEN G. LOUIE, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 — We present calculations of the quasiparticle energies and band gaps of graphene nanoribbons (GNRs) carried out using a first-principles many-electron Green's function approach. The self-energy of electrons is evaluated within the GW approximation. In our supercell calculation, due to the geometry of GNRs, a rectangular truncation of the Coulomb interaction is applied, which significantly improves the efficiency of the calculation. The quasiparticle results are compared and contrasted with results from previous studies that have been carried out either within the tight-binding or density functional formalism.

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Li Yang Dept. of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720

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