EDGE STATE EFFECTS IN MOLECULAR JUNCTIONS WITH GRAPHENE ELECTRODES

Dmitry A. Ryndyk\textsuperscript{1}, Jan Bundesmann\textsuperscript{2}, Ming-Hao Liu\textsuperscript{2}, and Klaus Richter\textsuperscript{2}

\textsuperscript{1}Institute for Materials Science and Max Bergmann Center of Biomaterials, Technische Universität Dresden, 01062 Dresden, Germany
\textsuperscript{2}Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

We consider plane junctions with graphene electrodes, which are formed by a single-level system (“molecule”) placed between the edges of two single-layer graphene half planes. We calculate the edge Green’s functions of the electrodes and the corresponding lead self-energies for the molecular levels in the cases of semi-infinite single-layer electrodes with armchair and zigzag edges. We show two main effects: first, a peculiar energy-dependent level broadening, reflecting at low energies the linear energy dependence of the bulk density of states in graphene, and, second, the shift and splitting of the molecular level energy, especially pronounced in the case of the zigzag edges due to the influence of the edge states. These effects give rise to peculiar conductance features at finite bias and gate voltages.