

The use of molecular junctions has shown a constant development in the miniaturization of electronic devices. Because, understanding electron transport plays a key factor to develop potential applications in nanoelectronic. Additionally, in most recent studies, the Green functions were used as a powerful formalism to study electronic transport across atomic junctions.

In this contribution, we involve an alternative model, based on the phase-field matching theory (PFMT) to investigate the electronic transport properties cross-molecular junctions. We focus on electric characterization and quantum scattering properties of Oligophenyl and Oligoacenes, both are examples of 1D-graphene nanoribbons. We show the impact of the PFMT by using a simple model system of two groups of semi-infinite monatomic chains of Gold (Au) or Silicon (Si), sandwiched together by molecular nanocontacts (Oligophenyl or Oligoacenes). The coherent transmission/reflection coefficients are calculated based on Landauer-Büttiker scattering matrix. The mathematical background of the PFMT is illustrated, we will consider the transport properties by using the Gold electrode instead of semi-infinite monatomic chains. In particular, we will investigate the effect of embedded atoms and magnetic fields across the molecular junction. The results exhibit an oscillation behavior of the transport properties under the presence of a magnetic field at the junction area