

MOLECULAR JUNCTIONS OF SILICENE AND GRAPHENE NANORIBBON: A STUDY BY DFT AND EHT/NEGF

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Abstract: The electronic transport in single-molecules donor-bridge-acceptor type it has been extensively studied since the Aviram and Ratner proposal. The steady decrease in the range of electronic materials has brought several advances to society, transforming smaller and more efficient devices. In this work we propose an investigation of the electronic properties of molecular junctions of ZigZag Silicene (ZZSiNR) and Graphene (ZZGNR) NanoRibbon by means of: Functional Density Theory (DFT) on the unit cell and Extended Hückel Theory / Non-Equilibrium Green Function (EHT / NEGF) using the Landauer-Buttiker formule for ZZSiNR and ZZGNR with 2 electrodes forming molecular junctions. Our results exhibit metallic behavior, a non-linear region for each nanoribbon with characteristic of a usual device (Field Effect Transistor, FET). These non-linear voltage regions coincide with the mínima voltage ($V_{\min}$) in the Fowler-Nordheim (FN) and Lauritsen-Millikan (LM) plots for molecular junctions of ZZSiNR and ZZGNR.

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