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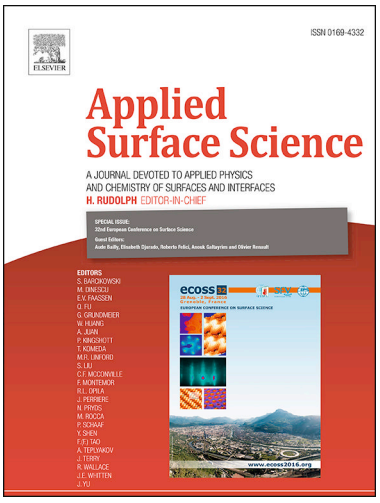

Full Length Article

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Graphdiyne Nanoribbon Based Diodes: A Theoretical Study on Rectifying Behavior of Nitrogen Doped Graphdiyne-Graphdiyne Heterojunction

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ABSTRACT

By applying non-equilibrium Green's functions (NEGF) in combination with tight-binding (TB) model, the electronic transport properties of heterostructures based on pristine and nitrogen doped armchair γ-graphdiyne nanoribbons (γ-A-GDYNRs) are studied under finite bias. Our results reveal that, in all n-type/semiconducting (n/s) ratios as the ribbon gets wider, the bandgap (E_g) becomes smaller and as a result the threshold voltage (V_{th}) decreases. It means that wider ribbons require smaller voltage to pass the current. Moreover, it is observed that as the n/s ratio in the central region of the device increases, more current passes through the device. This n-type/semiconducting junction shows a significant rectifying ratio (R). Furthermore, a big negative differential resistance (NDR) is observed as well. Transmission spectrum, band structure of electrodes and molecular projected self-consistent Hamiltonian (MPSH) are analyzed subsequently to more elucidate the electronic transport properties. Our findings could be used in developing nano scale rectifiers and NDR devices.

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