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Contemplating Charge Transport by Modeling of DNA Nucleobases Based Nano Structures

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Abstract : Electrical charge transport through two basic strands thymine and adenine of DNA have been investigated and analyzed using the jellium model approach. The FFT-2D computations have been performed for semi-empirical Extended Huckel Theory using atomistic tool kit to contemplate the charge transport metrics like current and conductance. The envisaged data is further evaluated in terms of transmission spectrum, HOMO-LUMO Gap and number of electrons. We have scrutinized the behavior of the devices in the range of -2V to 2V for a step size of 0.2V. We observe that both thymine and adenine can act as molecular devices when sandwiched between two gold probes. A prominent observation is a drop in HLGs of adenine and thymine when working as a device as compared to their intrinsic values and this is comparative more visible in case of adenine. The current in the thymine based device exhibit linear increase with voltage in spite of having low conductance. Further, the broader transmission peaks represent the strong coupling of electrodes to the scattering molecule (thymine). Moreover, the observed current in case of thymine is almost 3-4 times than that of observed for adenine. The NDR effect has been perceived in case of adenine based device for higher bias voltages and can be utilized in various future electronics applications.

Keywords : adenine, DNA, extended Huckel, thymine, transmission spectra
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