

## To expound superconductive quantum transport for C<sub>20</sub> fullerene with disparate electrode material

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**Abstract:** In this paper we expounded the optimal electrode material towards calculation of electron transport through fullerenes for the molecular electronics applications. We scrutinized the largest curvature fullerene, C<sub>20</sub> stringed to three variant semi-infinite electrode materials namely Copper, Silver and Gold at temperature of 0.100 K. The Geometry Optimization for the proposed configurations was completed using the Gaussian-03 and the optimized script was readied realizing tight binding semi-empirical Extended Hückel Theory (EHT) and Non-Equilibrium Green Function (NEGF) formalism for zero as well as variegated bias voltages. The various transport parameters thus elucidated for predicting the most optimal electrode material in such nanostructures. We perceived that the copper electrodes exhibited the transport properties comparable with that of gold, which had been the default choice for electrodes previously, while with silver electrodes, we found that though silver possesses the highest electrical conductivity in macrostructures, it exhibited the least conduction in nano configuration. The paper gives an insight on the use of copper electrodes for molecular junctions comprising of fullerenes.

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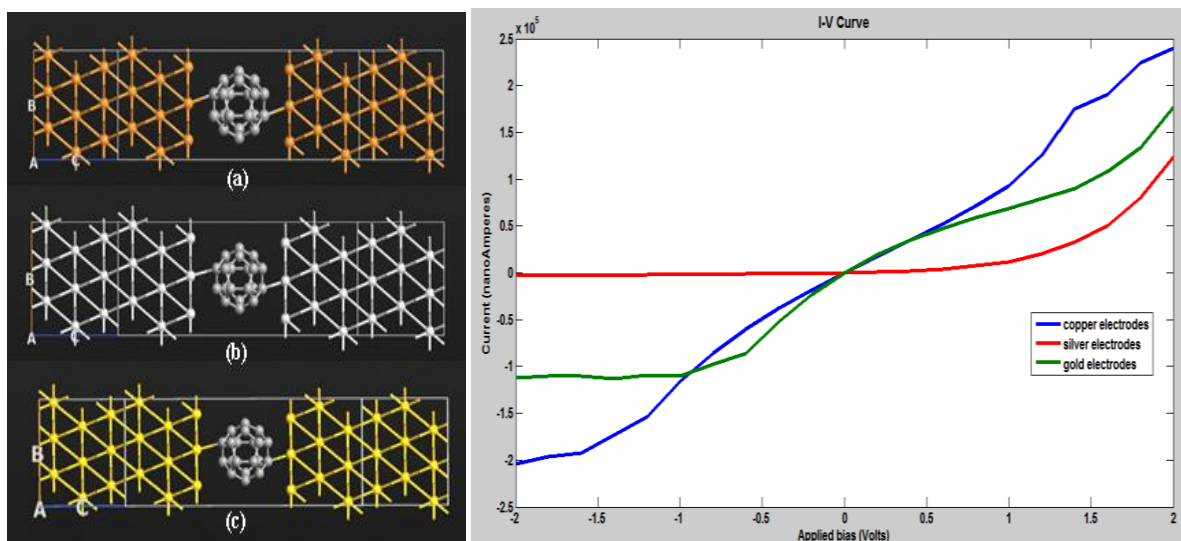
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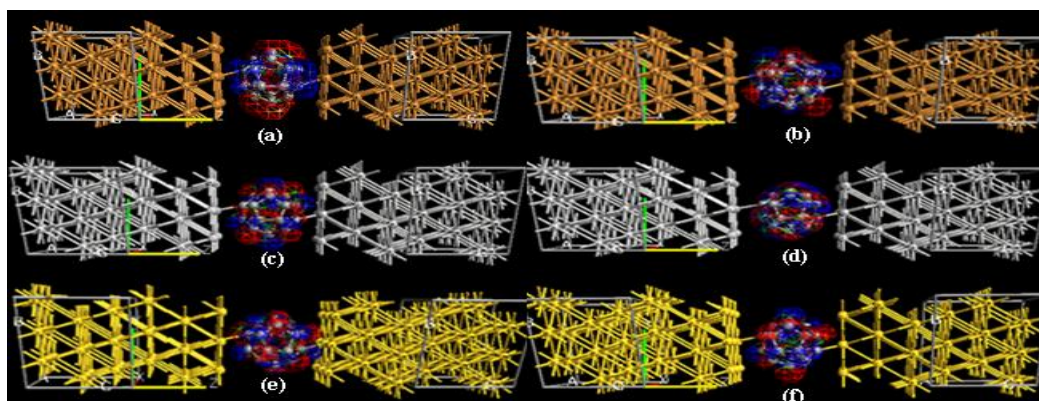
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**Figures**



**A.** C<sub>20</sub> stringed to electrodes

**B.** IV Curve



**C:** HOMO-LUMO at zero bias