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STUDY OF THE ELECTRONIC AND TRANSPORT PROPERTIES OF MELANIN USING DENSITY FUNCTIONAL THEORY (DFT)

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Organic semiconductors are relatively new member of semiconductor family and are composed of molecules containing carbon, hydrogen and other element. Melanin is the pigment that colours skin, eyes and hair and it could soon face a new generation of biologically friendly electronic devices in applications such as medical sensor and tissue stimulation treatment. Gaussian09 code, which uses density functional theory as working principle, was used to study electronic and transport properties of melanin structure. Three exchange functionals: HF (HF), GGA (PBE) and hybrid (B3LYP) were used at different basis set of 3-21G, 6-31G and 6-311G. It was found that at 6-311G level for the three exchange functionals of the total energy was -2981.03028, -2996.839821 and -3000.227297 eV respectively. However, the HOMO-LUMO energy gap was found to be 2.65 eV and is in agreement with the literature. Also information on IR and NMR (^{1}H and ^{13}C) were also reported.

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