Effect of chalcogendiazole groups on the conductive properties of EDOT containing polymers

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Tuning of the π-conjugated systems' backbone for the desired application is possible through modification of donor group as electron-rich or acceptor group as electron-deficient one. Electronic nature can be accomplished for the desired applications via changing the chalcogen atoms. In this work, impact of chalcogen atom substitution on electrochemical properties of semiconducting polymers was studied with density functional theory (DFT). A series of donor-acceptor-donor (DAD) systems with EDOT as an electron donor unit and benzoxadiazole, benzothiadiazole, benzoselenadiazole, benzotelluradiazole as electron acceptor units were investigated theoretically. Quantum chemical calculations are carried to calculate the HOMO-LUMO levels. For all conformations, B3LYP method was employed. Also, LANL2DZ and 6-31G(d) were used as basis sets. Obtained results indicate that the narrowest electronic band gap is achieved by introducing a heavy chalcogen atom, such as tellurium [1], into the donor and acceptor units of the semiconducting polymer. In the end, bandgap results are compared with the experimental findings in literature.

[1] Ozkilinc O, Kayi H, *Journal of Molecular Modeling*, **2019**, 25:167.

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