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Study on the optoelectronic proprieties and molecular structure of Alkyl-substituted Oligopyrrole for organic electronics HUSSAM BOUAAMLAT, OUFAE NINIS, MUSTAPHA ABARKAN, Laboratory of Engineering Sciences,Polydisciplinary Faculty,Sidi Mohamed Ben Abdellah University, Fes, Morocco, MOHAMMED BOUACHRINE, Superior School of Technology, Moulay Ismail University, Meknes, Morocco — The investigation of 3,3'-dicotylterpyrrole (DOTP), 3,3'-dihexylquaterpyrrole (DH4P) and 3,7-dimethyldienyloctyl-3'dodecylquarterpyrrole (ddoD4P) both in doped and undoped forms was performed on the basis of density functional theory (DFT) at B3LYP and UB3LYP/6-31G* level of theory. Alkyl-substituted Oligopyrrole is unique due to the presence of the alkyl as terminal, the structural and electronic proprieties along with infra-red spectra was investigated. the change in geometric parameters, and HOMO, LUMO, Gap energies analysis provide an effective evidence and suggest these compounds as good candidates for optoelectronic applications. Further support to the previous proprieties electronic excited state energies was extract by TD//B3LYP/6-31G(d). gap decreases as the oligomer chain length increases, illustrating that how electronic properties can be tuned by the backbone ring or side group. The results became more sophisticated in the doped form of ddoD4P.

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