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Charge transfer electronic states and reorganization energy of OLED α -NDP in amorphous and crystalline structure for organic electronics devices

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Renewable energy alternative promising with organic photovoltaic cells convert sunlight into electricity. They are several polymeric materials that are light, flexible, inexpensive to manufacture and adjustable at molecular level. To this end, an investigation of charge transport by ADF/PBE0/DZ and TD-DFT quantum methods in the molecule-to-molecule hopping regime through charge transfer integrals and reorganisation energies was performed on an OLED α -NPD semiconductor in amorphous and crystalline structure, exposing its optoelectronic properties in aggregate configurations. For each α -NPD configuration with 1050 isolated monomers molecules, the transfer integrals of more than 10.000 dimers were determined and rationalised by overlapping HOMO or LUMO orbitals, for both hole and electron transport. The comparison of the average charge transfer integrals in the two structures suggests that holes move as fast in amorphous structure then in crystalline structure, which allows to propose in the performance the aggregate in amorphous structure for Organic Electronic Devices.

Key Words: OLED α -NPD, ADF/PBE0/DZ, Amorphous and Crystalline Structure.

Biography

Simplice Koudjina has been working as an Assistant Professor in Chemistry at the National University of Sciences, Technology, Engineering and Mathematics (UNSTIM) in Benin, where he works since 2019. He holds a Ph.D. degree in Theoretical Chemistry and Molecular Surface Modeling at the University of Abomey-Calavi since 2016. He obtained M.Sc. in Nanotechnology at the University of Namur in Belgium. He then joined the research group of Professor, Guy Sylvain Y. Atohoun in the Laboratory of Theoretical Chemistry and Molecular Spectroscopy (LACTHESMO) at University of Abomey-Calavi (UAC) in BENIN REPUBLIC. At 2022, he has obtained a Postdoc research stay in the group of Professor in Department of Chemistry at National Institute of Technology (NIT) Kurukshtra – INDIA. His field of expertise is computational Chemistry and Molecular Surface Modeling. He has published more than 20 research articles in impact factor journal.

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