Centre d'Etudes Doctorales : Sciences et Techniques de l'Ingénieur

AVIS DE SOUTENANCE

THESE DE DOCTORAT

Présentée par

Mr: HUSSAM BOUAAMLAT

Discipline : Physique

Spécialité : Physique des Matériaux et Nanostructures

Sujet de la thèse : New Organic Materials Based on Ethylcarbazole For Optoelectronic Applications : Characterization and computational studies.

Formation Doctorale : Sciences de l'ingénieur, Sciences Physiques, Mathématiques et Informatique.

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Etablissement : Faculté Polydisciplinaire de Taza.

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Nom du candidat : Hussam BOUAAMLAT
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Résumé de la thèse

Organic electronics is a rapidly expanding field that has recently developed around organic materials based on pi-conjugated molecules. In this context, the thesis covers theoretical and experimental approaches to deal with such materials for optoelectronic applications. This work represents an effort to understand the key parameters that can improve their performance. A study was applied on Polypyrrole based material to examine the effect of the elongation of the 3,3'-dioctylterpyrrole (DOTP) and 3,3'- dihexylquaterpyrrole (DH4P) on the geometric, electronic and absorption properties, as well as the influence of alkyl chain in 3,3'- dihexylquaterpyrrole (DH4P) and 3- 3,7– dimethyldienyloctyl-3'dodecylquaterpyrrole (ddoD4P). Next, seven dye sensitizers based on Selenophene as a p-spacer, besides multiple electron-donating groups, were used with 2-cyanoacrylic as an electron acceptor unit forming D-pi-A structure. We discussed structural and electronic properties alongside with the dependency of the photovoltaic parameters (open-circuit voltage (Voc), oxidation potential energy, and electron injection force), in order to find the potential sensitizers for DSSCs applications. Thus, Density Functional Theory (DFT) and Time-Dependent DFT (TDDFT) was carried out with many functionals and basis sets. For the bulk Ethylcarbazole-based materials, the same theoretical procedures mentioned above were adopted. Regarding the experimental part, characterization measurements involved different techniques such as X-ray diffraction, scanning electron microscopy and UV-Vis was used to gain insight into the structure of the materials. Then, the dielectric and electrical properties have been studied over the frequency range from 1 kHz to 2 MHz, and the temperature range from 30 ◦C to 120 ◦C, to explore the effect of changing the polymer blocks in our material.