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Structural and Electronic Properties of the Fuorophore 9,10-Bis(Phenylethynyl)Anthracene (Bpea) for Organic Solar Cells

R.Kacimi[1], T.Abram[1], A. El alamy[2], L. Bejjit[1] and M. Bouachrine[1*]

1. MEM, High School of Technology (ESTM), University Moulay Ismail, Meknes, **MOROCCO**
2. LCBAE/CMMBA, Faculté des Sciences, Université Moulay Ismail, Meknes, **MOROCCO**

Email: bouachrine@gmail.com

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ABSTRACT

The search for renewable energy currently leads the development of photovoltaic cells where organic conductive materials can play a vital role due to their ability to separate the electron-hole pairs and carry these loads to the electrodes in specific electronic configurations. In this work, a quantum chemical investigation has been performed to explore the optical and electronic properties of a series of different compounds based on BPEA. The structures are studied by means of quantum chemical calculations based on density functional theory (DFT) using B3LYP functional with 6-31G (d,p) for all atoms and all states (ground and doped). The study of the geometrical parameters, ground and doped states (p, n) showed that the structures of these oligomers are planar. Different electron side groups were introduced to investigate their effects on the electronic structure. The theoretical knowledge of the HOMO and LUMO energy levels of the components is basic in studying organic solar cells. So, the HOMO, LUMO, Gap energy and the photovoltaic properties of the studied compounds have been calculated and reported. These properties suggest these materials as good candidates for organic solar cells.

Keywords: Photovoltaic cells, DFT, Thiophene, organic solar cells.