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# Study of Excited States of Polycyclic Aromatic Hydrocarbons (PAHs)

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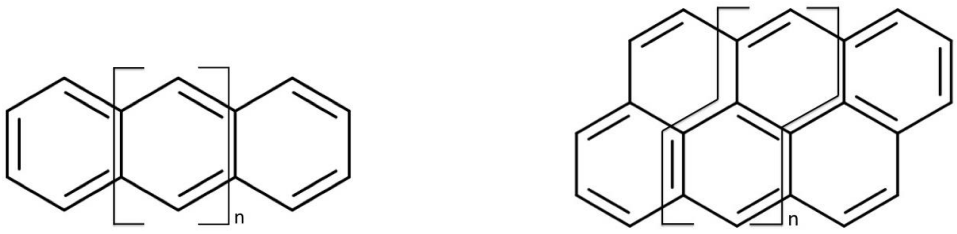
Polycyclic aromatic hydrocarbons (PAHs) have been used as graphene's model of electronic structure characterization [1]. Since the initial graphene experiments, it has been used in several areas, such as sensors manufactory, organic semiconductors, spintronic and non-liner optics and the study of its electronic structure is very important for these applications [2]. Therefore, the characterization of the fundamental and excited electronic states of PAHs, n-acenes (Figure 1a) and periacenes (Figure 1b) is the main goal of this work.




(a) (b)

Figure 1. (a) Structure of studied acenes (n=0-4) and (b) periacenes (n=0-4)

Molecular quantum chemistry methods are highly used in PAHs studies. In this work, the Time-Dependent Density Functional Theory (TD-DFT) was employed with M06-2X and WB97-XD functionals and 6-31G* basis set. The absorption spectra calculations were performed to describe the two lower singlet energy excitations that correspond to the La and Lb bands of acenes (Figure 2) and periacenes (Figure 3). Properties as the character of the transition and the involved orbitals were analyzed. The La band consists in a single HOMO→LUMO excitation while Lb band consists in two single excitations: HOMO-1→LUMO and HOMO→LUMO+1. La band present an ionic character and Lb, covalent character. La band was good described by both tested functionals presenting results close to experimental data. Lb band is harder to be described but both functionals present the same tendency as the experimental data.

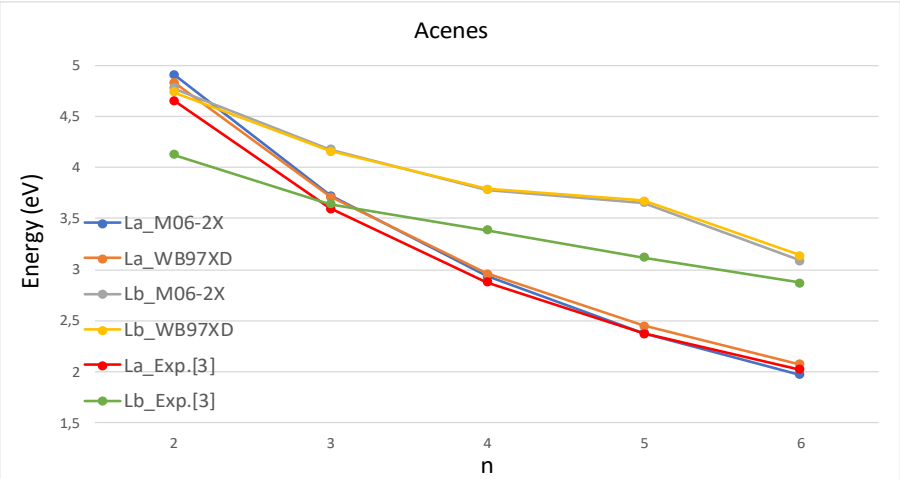



Figure 2. La and Lb band energies for all acenes studied calculated with M06-2X and WB97XD and experimental [3].

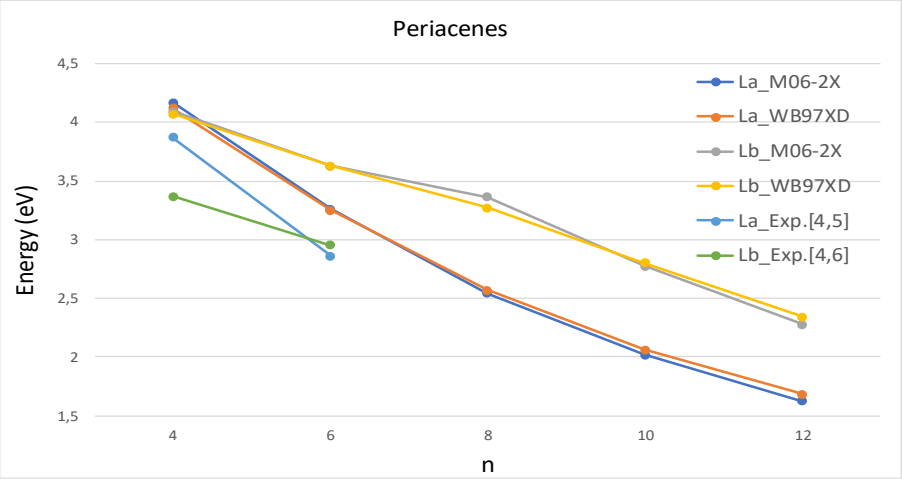



Figure 3. La and Lb band energies for all periacenes studied calculated with M06-2X and WB97XD and experimental [4-6].

**Key-words**: Acenes, periacenes, excited states, TD-DFT.
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