Systematic study on charge transport and spectroscopic properties: A DFT Benchmark of LCD's molecules

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Introduction

Nowadays we have been faced with a large quantity of papers, works and device due the technological improvements of TV's and monitors, OLED's and LCD's, in the last years[1]. So, in this work we have been investigated LCD's molecules focusing the development of a database of electron/hole transfer and spectroscopic properties[2,3]. In this sense, a DFT benchmark has been created to evaluate these properties that have a large dependence of functionals and basis sets.

Methodology

We have been chosen M06-2X, w-B97XD, CAMB3LYP and B3LYP functionals and 6-31+G*, 6-31+G** basis sets to describe molecules based in branched mesoionic centers to generate a discotic-like molecular electronic devices[4] considering Alq₃ such as the reference molecule[2,3].

Results

Figure 1: Results of Lambda (electron or hole) to B3LYP/6-31+G*.

Discussion

In figure 1, all the molecules shown reasonable results to electron transfer properties when compared with Alq₃ reference, with lambda hole and electron one greater than 1.2 times than that.

Conclusions

Through these data, we could modeling molecules that could employed in this study to be great candidates to best electron/hole transfers new materials.

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