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Optoelectrical, electronic and thermodynamic DFT study of a carbon nanoring and its derivative – HPC application as a computational chemistry resource

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INTRODUCTION

PURPOSE

❑ Study the Optoelectrical, Electronic and Thermodynamic properties of {6}cycloparaphenylene ({6}CPP) and its derivative for potential application in Organic solar cell (OSC) and non-linear optics (NLO).

Engagement

- To overcome the current limits of current OSC Structures By seeking alternative materials with more challenging properties.

Outcomes

➢ We are expecting very promising results obtained from Gaussian 16 program, the calculation of the properties of ({6}CPP) and its derivative, that show this material is an excellent candidate for OSC and NLO efficiency improvement.

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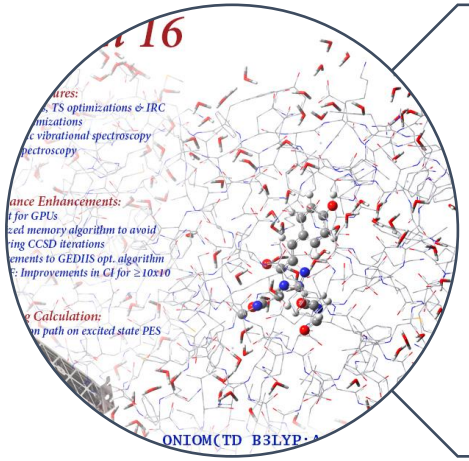
METHOD

Thanks to the **HPC resources**, computational chemistry suite of program **Gaussian 16**



Density functional theory (DFT) and Time-dependant DFT (TD-DFT)

- APFD and B3LYP functionals with Grimme Dispersion (D3)
- split
  valence balanced 6-311++G(*d,p*) Pople basis set

Method of inquiry

- **Gaussian codes**

METHOD

Gaussian code

- **DFT calculations**
  - # B3LYP 6-311+g(d) opt freq scf(maxcycle=999,xqc)
  - # APFD 6-311+g(d) opt freq scf(maxcycle=999,xqc)
  - # B3LYP 6-311+g(d) polar scf(maxcycle=999,xqc)
  - # APFD 6-311+g(d) polar scf(maxcycle=999,xqc)
  - # B3LYP 6-311+g(d) polar scf(maxcycle=999,xqc)
- **TD-DFT calculations**
  - B3LYP 6-311+g(d) TD (nstates=70) scf (maxcycle=999,xqc)

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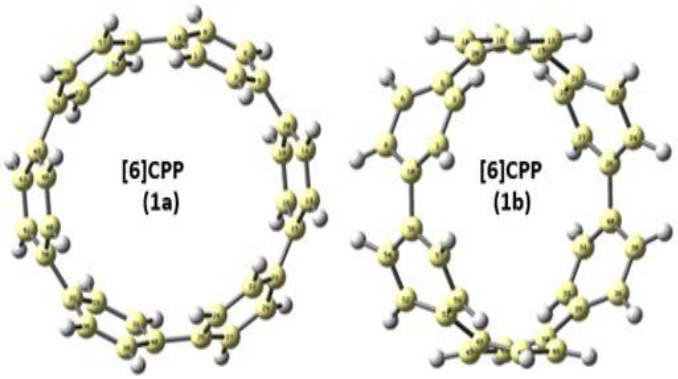
METHOD

Mathematical model

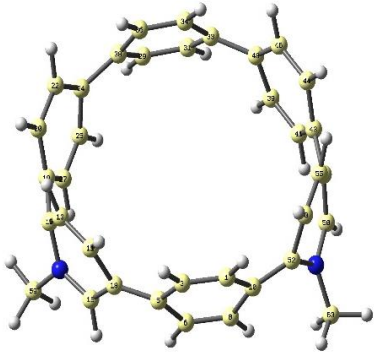
- Very complex level of theory calculations with Gaussian 16 of CHPC



Optical and non-linear optical calculations

$$\alpha = \left(\frac{1}{3}\right)(\alpha_{xx} + \alpha_{yy} + \alpha_{zz})$$

$$(\Delta\alpha)^2 = \frac{1}{2}\left[(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{zz})^2 + (\alpha_{zz} - \alpha_{xx})^2\right] + 3\left[(\alpha_{xy})^2 + (\alpha_{xz})^2 + (\alpha_{yz})^2\right]$$



$$\beta = \left[\left(\beta_{xxx} + \beta_{xyy} + \beta_{xzz}\right)^2 + \left(\beta_{yyy} + \beta_{yxx} + \beta_{yzz}\right)^2 + \left(\beta_{zzz} + \beta_{zxx} + \beta_{zyy}\right)^2\right]^{\frac{1}{2}}$$

Thermodynamic calculations

$$S = N_A k_B + N_A k_B \left(\ln(q_t q_e q_r q_V) + T\left(\frac{\partial \ln(q_t q_e q_r q_V)}{\partial T}\right)_V\right), \quad \mathrm{E}_{tot} = 3RT + R\sum_K e^{\Theta_{V,K}/T}\left(\frac{\Theta_{V,K}/T}{e^{-\Theta_{V,K}/T} - 1}\right)^2$$

$$\mathrm{H}_{corr} = \mathrm{E}_{tot} + k_B T \qquad \mathrm{G}_{corr} = \mathrm{H}_{tot} - TS_{tot}$$

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RESULTS & CONCLUSION

Opto-electrical and electronic properties

- Band gap 3.1 eV and 1.38 eV, $\varepsilon_r = 5{,}69\ eV$ $\chi_e = 4{,}69\ eV$, $E_b^{exc} = 0{,}18eV$, LHE= 25%
- hole/electron reorganisation energy ratio 0.78 → P conductivity

Optical and non linear optical properties

- $\alpha_0(\{6\}CPP) = 456.1$, $\alpha_0(DMDA\{6\}CPP) = 646.8$ a.u
- $\beta(DMDA\{6\}CPP) = 10195.8$ a.u

Thermodynamic properties

- Stable compounds

We thanks the **HPC resources**, **Gaussian 16 program.**

Our relating article has been **accepted on the November 09, 2022.**