Absorption Spectrum and Charge Transfer effects in dicyanovinyl-substituted quarterthiophene (DCV4T)/C60 materials for organic solar cells

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INTRODUCTION

Renewable energy sources is nowadays a necessity. For this reason, developing new materials for converting light into electricity via photovoltaic effect is an increasingly important scientific field. Organic solar cells made of conjugated polymers are promising materials due to their low cost and flexibility. However, their fundamental electronic processes are still not clearly understood.

In this work, we investigate a promising polymeric material, the bulk heterojunction (BHJ) combining donor dicyanovinyl-substituted quarterthiophene (DCV4T) and acceptor fullerene C_{60}.[1] For seven different conformers of this BHJ, the absorption spectrum and charge transfer effects in excited states were investigated.

METHODS

Time-dependent density functional theory (TDDFT) with the PBE functional and the SV(P) base set were used to fully optimize the structures and compute the electronic spectrum. The algebric-diagramatic method to second order - ADC(2), an ab initio wave function, was also used and successfully employed before in similar systems.[2] The software Turbomole 6.6 was used for all calculations.

RESULTS AND DISCUSSION

Figure 1 shows the so called DH configuration, the lower energy one.

The energy difference between the seven conformers is small: the largest was 4 kcal/mol. To illustrate the computed results, Table 1 displays data from 5 out of the 7 studied structures.

Configurations	DH	DN	TiS	Tiot	Tit
Relative (kcal/mol)	0.0	3.79	3.46	3.57	3.82
Gap (ev)	1.20	1.37	1.05	1.26	1.24
First excitation	1.21	1.41	1.06	1.26	1.24

Table 1. Computed PBE/SV(P) properties of five out of seven studied structures.

The computed relative energies excepting the lower energy DH structure are very close. The gap calculated as the HOMO-LUMO energy difference has a very good agreement with the PBE excitation energies, hence indicating the dominant single configuration character of this state.

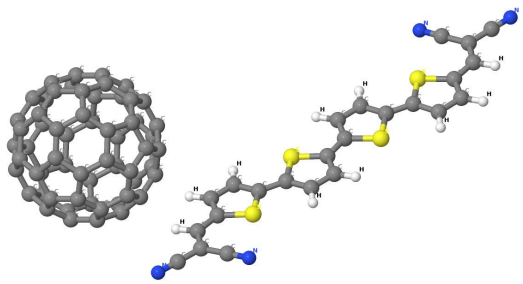

Figure 1. PBE/SV(P) converged DH conformer.

CONCLUSIONS

ADC(2) calculations are underway and will compared with PBE results. The charge transfer character of the first excited states, which are of interest for organic solar cells, are being quantified.

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