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Interchain Coupling Effects in Parallel Bithiophene Dimers: A Theoretical Study

Oumaima El ouardi, Brahim Fakrach, and Hassane Chadli.

Laboratory of Advanced Materials Study and Applications (LEM2A), Moulay Ismail University, Faculty of Sciences, BP 11201, Zitoune, Meknes, 50000, Morocco.

INTRODUCTION & AIM

Conjugated organic materials have attracted significant attention in recent years due to their structural flexibility, low production cost, and tunable optoelectronic properties. Among these materials, parallel bithiophene dimer–based systems stand out as promising candidates for organic electronic and photovoltaic devices, such as solar cells, photodetectors, and field-effect transistors.

The electronic and optical behavior of these compounds is largely determined by the degree of π-conjugation and the arrangement of molecular units. In particular, the interaction between parallel bithiophene chains can lead to enhanced π–π stacking, improved charge carrier transport, and strong light–matter interactions, which are crucial factors for efficient energy conversion in optoelectronic applications.

The main objective is to evaluate their band gap, semimetallic behavior, and absorption performance in the visible region, highlighting their potential for organic photovoltaic and photodetector applications.

METHOD

Computational method:

Electronic properties

The electronic and optical properties of **Parallel Bithiophene Dimers** were investigated using **DFT (VASP)** with geometric optimization (residual forces < 0.02 eV/Å). The calculations employed:

- PBE (GGA) functional
- 520 eV energy cutoff
- Monkhorst-Pack (1×1×1) k-point grid
- PAW-PBE pseudopotentials

This approach enables precise characterization of electronic properties for **optoelectronic applications.**

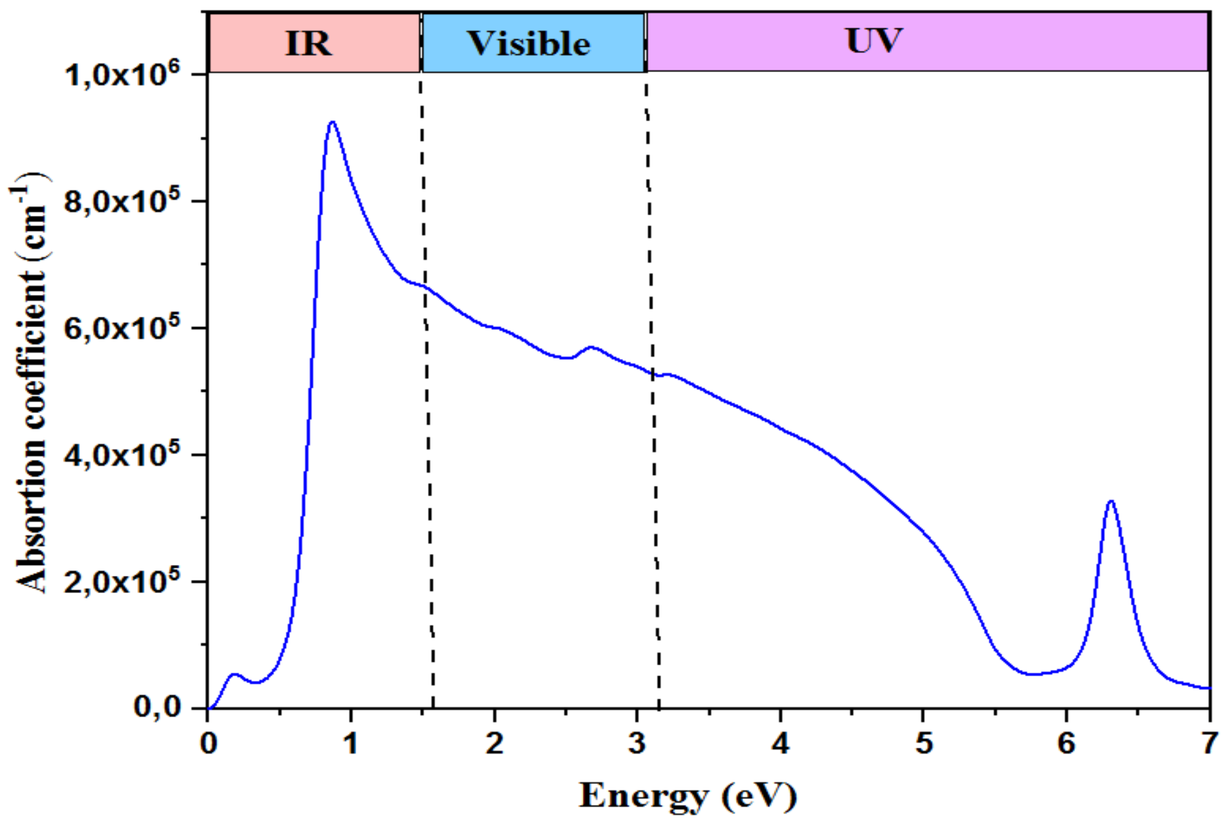
RESULTS & DISCUSSION

Electronic properties

Table 1. Energy levels of HOMO and LUMO, Fermi level (Ef) and HOMO-LUMO gap (Eg) of **Parallel Bithiophene Dimers** in eV.

	HOMO	LUMO	Eg	E_f
2T-2T	-4.2936	-4.2886	0.0051	-4.2911

Optical properties



CONCLUSION

The study of **Parallel Bithiophene Dimers** shows that they combine a very small band gap, indicating a semi-metallic behavior, with a high absorption coefficient in the visible and UV regions. These features demonstrate excellent electronic conductivity and a strong light-harvesting capability, highlighting their potential as efficient materials for organic photovoltaic applications and photodetection devices. These results pave the way for exploring these dimers in the development of new optoelectronic technologies.

FUTURE WORK / REFERENCES

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