IOCEN 2026 Conference

The 3rd International Online Conference on Energies

12–15 May 2026 | Online

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Unveiling the Role of Donor-Acceptor Attachment Sites in Molecular Design for High-Performance Organic Solar Cells: A Theoretical Study

Sana Abbas[1], Usman Ali[2], Abdessamad Tounsi[1]

[1]Sultan Moulay Slimane University, Morocco
[2]University of Rome Tor Vergata, Italy

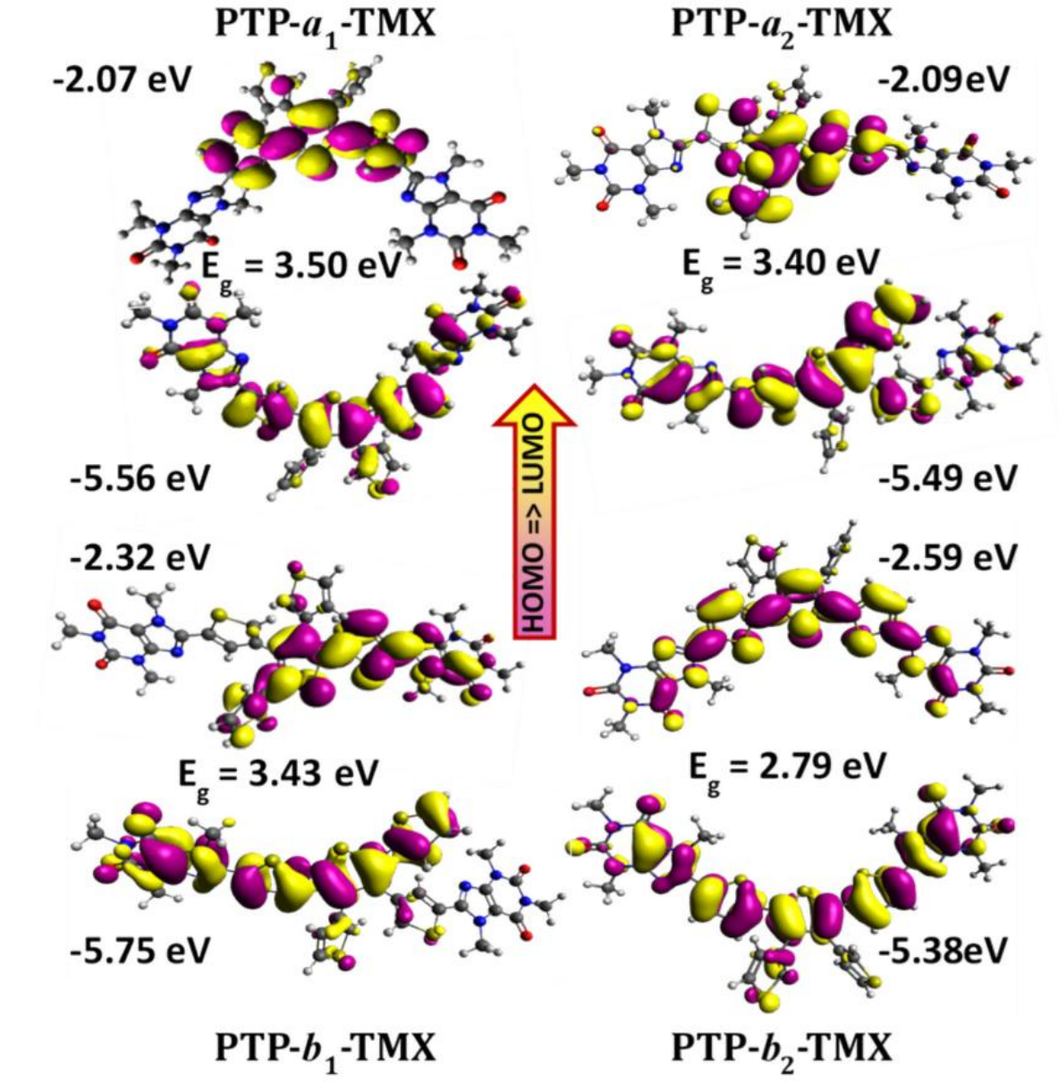
INTRODUCTION & AIM

Small-molecule organic solar cells can be tuned by donor-acceptor molecular engineering. This work tests a controlled design idea: keep the same PTP donor core and TMX terminal acceptors but vary only the attachment positions. The aim is to reveal how connection topology controls optoelectronic and photovoltaic descriptors.

COMPUTATIONAL WORKFLOW

Gaussian 16 calculations were performed at B3LYP/6-31G(d,p). TD-B3LYP/6-31G(d,p) with PCM/THF was used for excited states. Key descriptors included HOMO/LUMO, Eg, λmax, oscillator strength, LHE, electron/hole reorganization energies, VOC, FF and estimated PCE.

FRONTIER ORBITALS

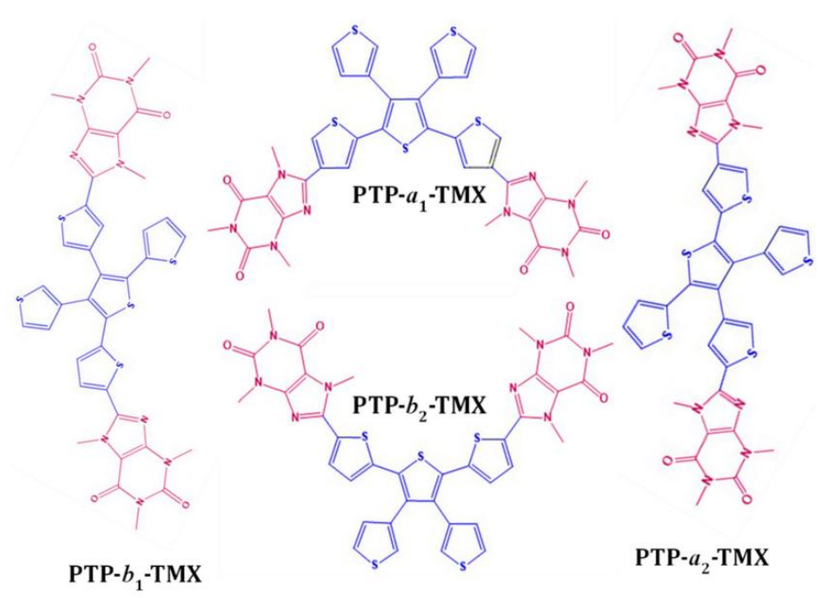


PTP-b2-TMX shows the narrowest gap (Eg = 2.79 eV), supporting stronger ICT and easier photoexcitation.

MAIN CONCLUSION

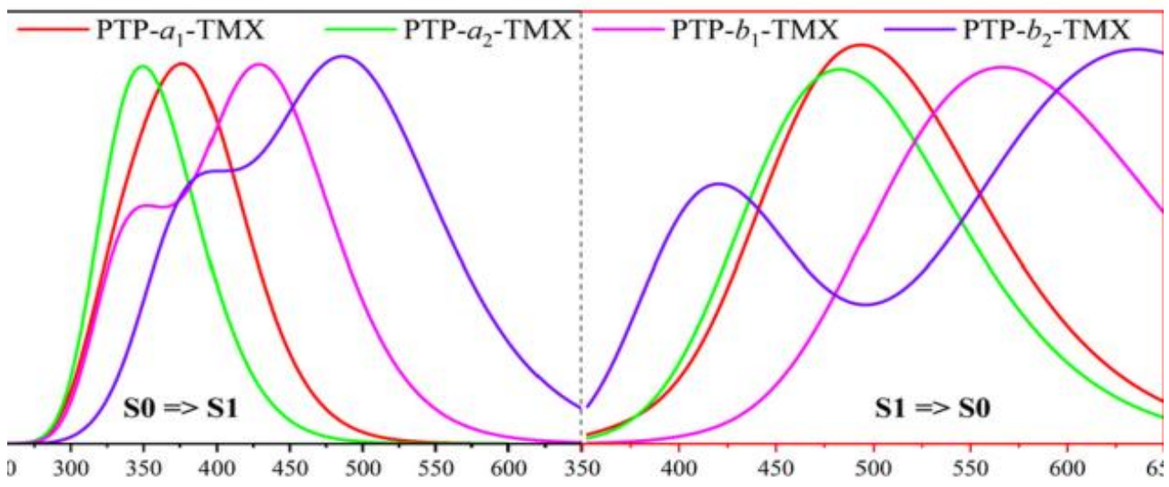
- Attachment position is not a minor structural detail; it changes optical absorption, orbital distribution and charge transport.
- PTP-b2-TMX is the best photophysical/transport molecule: λmax = 491.82 nm, LHE = 0.96 and λh = 0.30 eV.
- PTP-b1-TMX gives a strong balanced photovoltaic profile with PCE = 3.56%, VOC = 3.71 V and LHE = 0.94.
- The most useful design rule is balance: absorption, voltage and mobility must be optimized together.

MOLECULAR DESIGN



Four isomeric A-D-A molecules: PTP-a1-TMX, PTP-a2-TMX, PTP-b1-TMX and PTP-b2-TMX.

OPTICAL RESPONSE

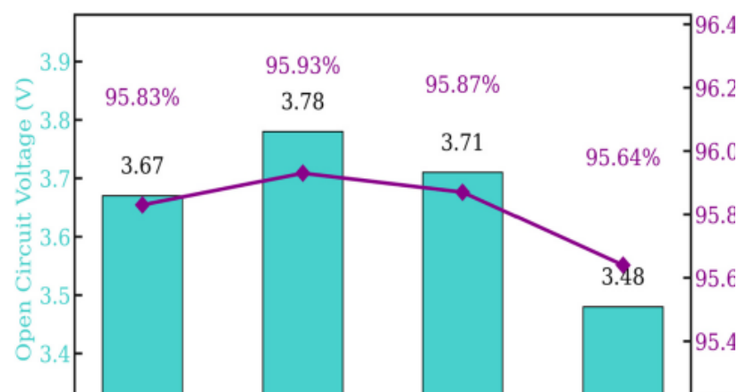


Red-shift order: PTP-a2-TMX < PTP-a1-TMX < PTP-b1-TMX < PTP-b2-TMX. The b-series absorbs further into the visible region.

KEY PERFORMANCE INDICATORS

2.79 eV	491.82	0.96	3.56%
lowest Eg PTP-b2-TMX	λmax (nm) PTP-b2-TMX	highest LHE PTP-b2-TMX	balanced PCE PTP-b1-TMX

PHOTOVOLTAIC DESCRIPTORS



The theoretical PCEs are comparative molecular descriptors, not final device efficiencies. PTP-a2-TMX gives the highest numerical model PCE (3.63%), but PTP-b1-TMX offers the stronger overall balance of VOC, LHE and PCE.

FUTURE WORK / REFERENCES

Next steps: explicit blend modelling, solid-state packing, morphology, exciton diffusion and device-level validation.

Reference: S. Abbas et al., Computational and Theoretical Chemistry 1256 (2026) 115639. DOI: 10.1016/j.comptc.2025.115639.