

A low-cost thiophene-based hole transport material containing azomethine as a bridge for perovskite solar cells or absorber organic solar cells: a Theoretical study

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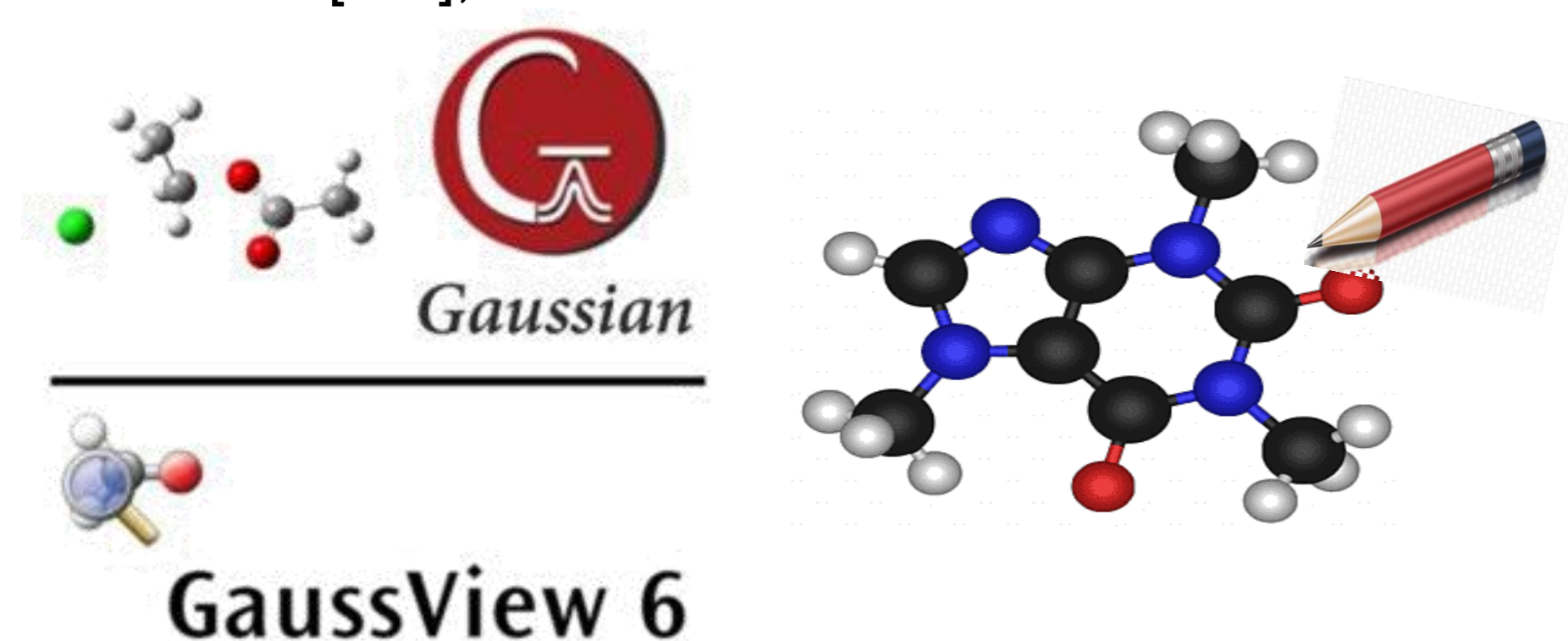
INTRODUCTION & AIM

Perovskite solar cells (**PSCs**) represent one of the most rapidly advancing areas in renewable energy research, with their power conversion efficiency (**PCE**) increasing from less than 5% in 2009 to a certified value exceeding 27% by 2025 [4]. A key component of PSCs is the hole transport material (**HTM**), and numerous HTMs have been synthesized to date [2]. Due to their tunable optoelectronic properties and ability to enhance PCE, organic photovoltaic materials have attracted considerable interest. The design and optimization of HTMs remain central to further improving PSC performance.

In this study, four novel **D- π -A- π -D** type HTMs (**H1–H4**) were developed by modifying the acceptor core of a previously synthesized reference molecule (**HR**). Their optical and quantum chemical properties were investigated through computational simulations. Theoretical results were further supported by experimental validation, demonstrating that all four proposed HTMs exhibit superior photovoltaic potential compared to the reference structure, with enhanced capability for solar energy conversion.

METHOD

- ❑ Density functional theory (DFT) using the hybrid density functional named Becke's three-parameter exchange functional (B3LYP):
- ❑ The optimization and electronic properties of the designed HTMs were performed using the DFT and TD-DFT methods [1-3],



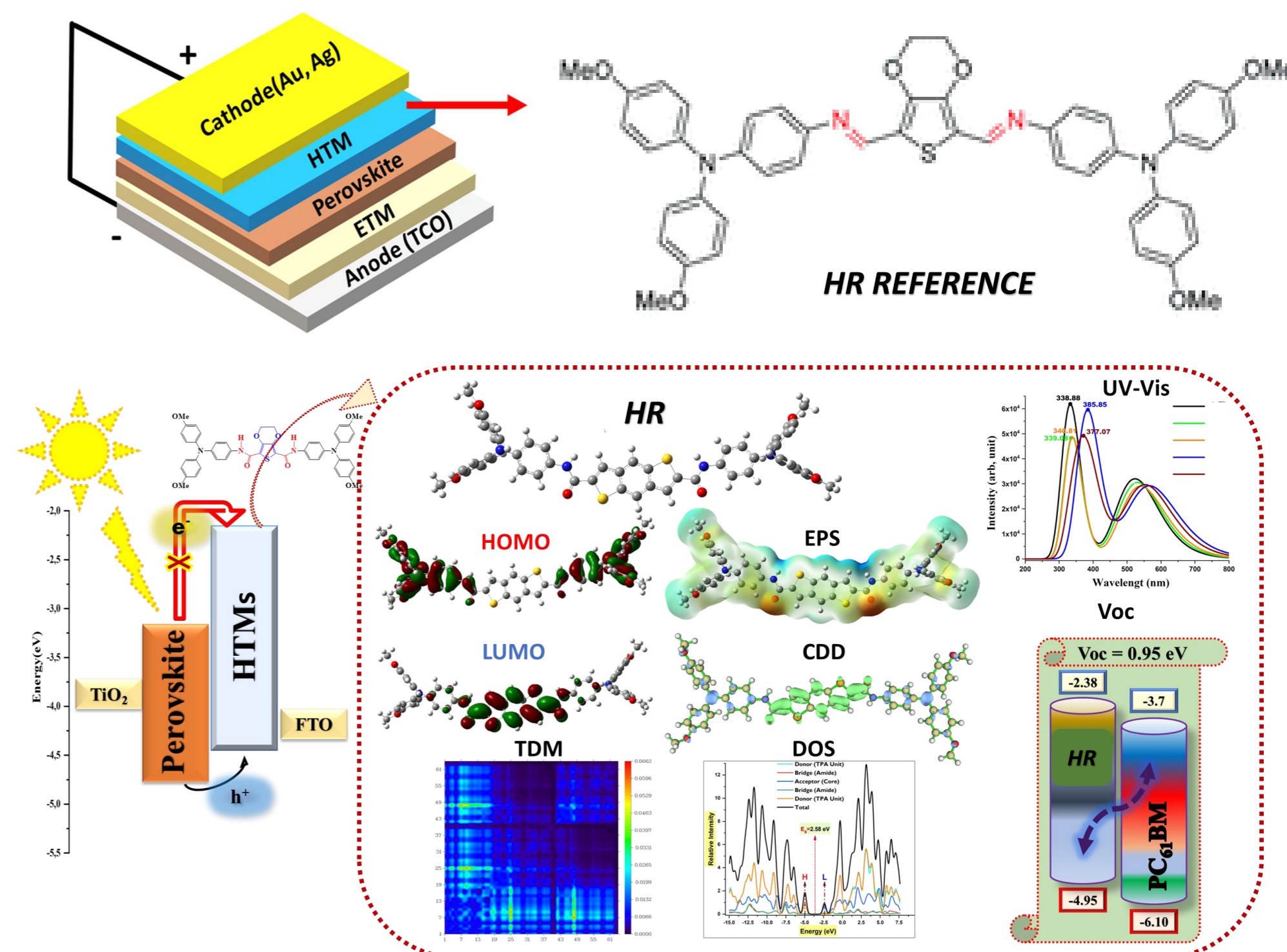
Drawing and visualization of the systems studied

All calculations were performed using the Gaussian 16 program,



Drawing and visualization of the systems studied

RESULTS & DISCUSSION



For application in perovskite solar cells (PSCs), four thiophene-based organic compounds with amide bridges, TPA side groups, and various thiophene central cores were created as D- π -A- π -D type HTMs. Intermolecular charge transfer is positively impacted by the designed compounds H1–H4. Their IP and EA values, along with their superior FMOs delocalization, show that these structures have promising prospects for improving charge mobility and performance. They are excellent candidates for HTMs in perovskite solar cells due to their lower hole reorganization energies, longer radiative lifetimes, improved light-harvesting efficiency, and spontaneous solvation in DCM. These molecules' bonded electron-hole pairs easily separate into positive and negative charges, which promotes hole transport and may raise the density of short-circuit current. H1–H4 show greater Stokes shifts than spiro-OMeTAD, which is beneficial for pore-filling HTMs in PSCs. Extremely powerful ICT is demonstrated by the core's H3 and H4 groups. The longest radiative lifetimes are shown by H1 and H4, but H3 and A4 have superior CT from D to A regions. Because of their minimal spatial overlap of holes and electrons, which enabled efficient charge separation, when paired with the acceptor molecule PC₆₁BM, H4 emerged as the most promising candidate, demonstrating a lower band gap, higher maximum absorption, and exceptional photovoltaic properties,

In conclusion, this study strongly recommends the synthesis of these high-performance materials for future research applications.

CONCLUSION

- ✓ DFT/TD-DFT calculations were performed on various HTMs,
- ✓ **HR**-based HTMs were designed for use in PSCs,
- ✓ The HOMO energies of all HTMs were higher than those of the perovskite,
- ✓ All HTMs **H1-H4** exhibited a higher V_{OC} than that of the AR reference,
- ✓ Almost all HTMs showed good charge transfer, along with higher dissociation rates and lower charge coupling,

FUTURE WORK / REFERENCES

- [1]** A, Staoui, A, Idrissi, Z, Elfakir, Said Bouzakraoui, Journal of Photochemistry & Photobiology, A: Chemistry 453 115630 (2024),
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