Fusing together Nitrogen-rich Building Blocks to Design New Quinoxaline based Non-fullerene Electron Acceptors for Organic Photovoltaics

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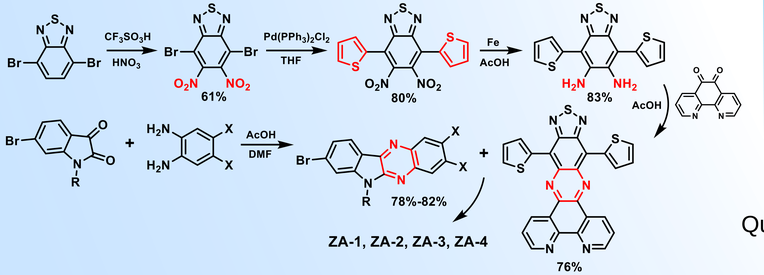
Introduction

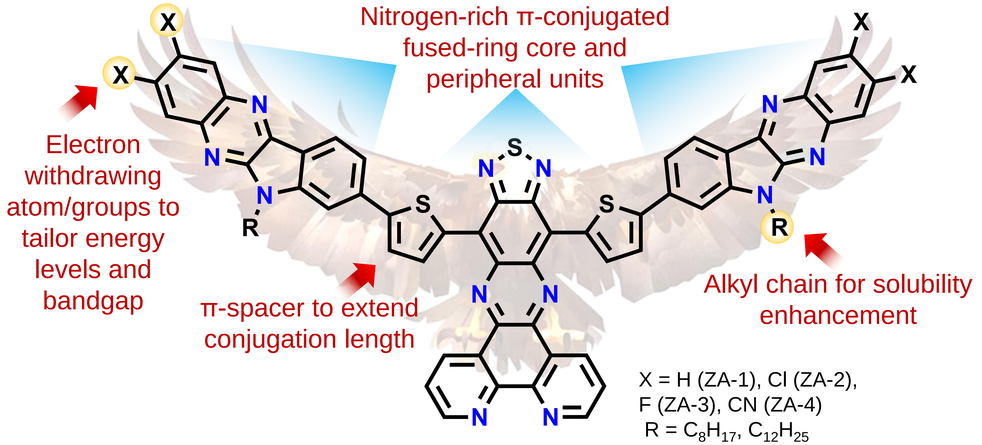
Organic Solar Cells (OSCs) are amongst the most promising renewable energy conversion solutions. Combining the features of low-cost and flexibility, OSCs are idealized for portable electronic devices, indoor light-harvesting applications and building-integrated photovoltaics. Fused-ring non-fullerene electron acceptors have frequently exhibited champion power conversion efficiencies owing to a well-connected π-conjugated framework which enables higher light absorption and electron charge transfer.[1-3] Herein, we introduce new non-fullerene acceptors containing a benzothiadiazole unit fused with 1,10-phenanthroline through the phenazine moiety and flanked with indolo[2,3-b]quinoxaline derivatives.

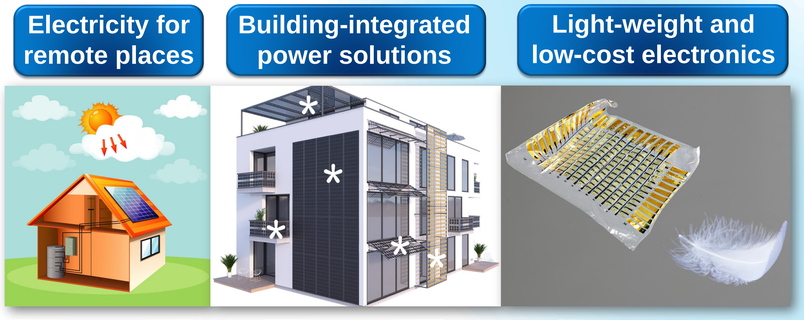
1. Bi, P. et al., *Joule* **2021,** *5* (9), 2408-2419.
2. Holliday, S. et al., *JACS* **2015,** *137* (2), 898-904.
3. Yue, W. et al., *Advanced Materials* **2015,** *27* (32), 4702-4707.

Synthesis

Molecules have been synthesized using established methodologies considering high scalability and reproducibility.







Computational Studies

Calculations performed on Gaussian 09, using DFT B3LYP(d,p) method and 6311g basis set revealed the possibility of band gap engineering by the introduction of halogen atoms on the periphery, thus allowing structure tuneability for optimum photovoltaic performance.

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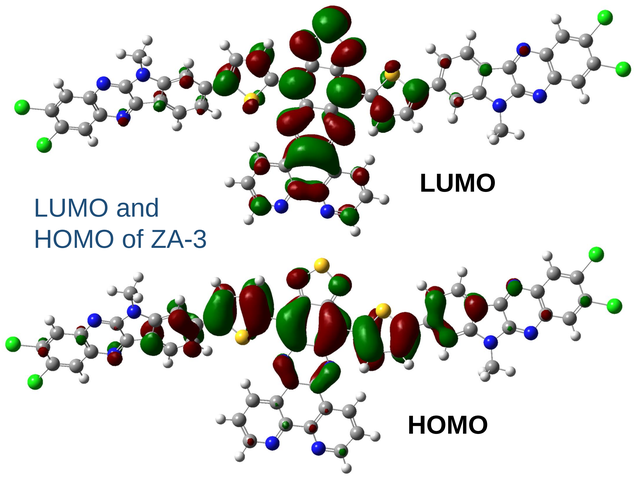
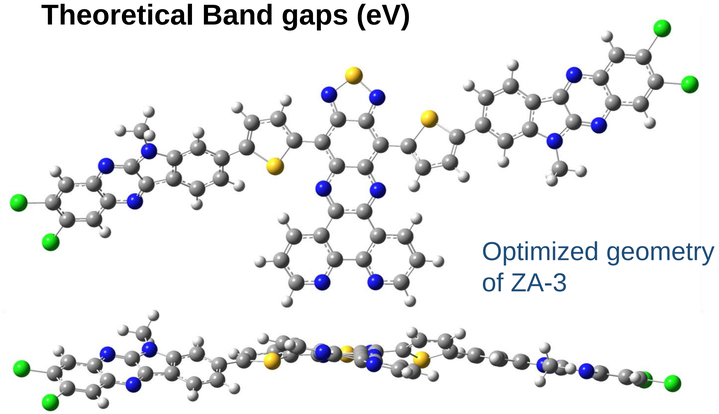
Queen Mary Apocrita HPC System
NRPU, HEC, Pakistan



ZA-1	ZA-2	ZA-3	ZA-4
2.24	1.60	1.56	1.62

Theoretical Band gaps (eV)