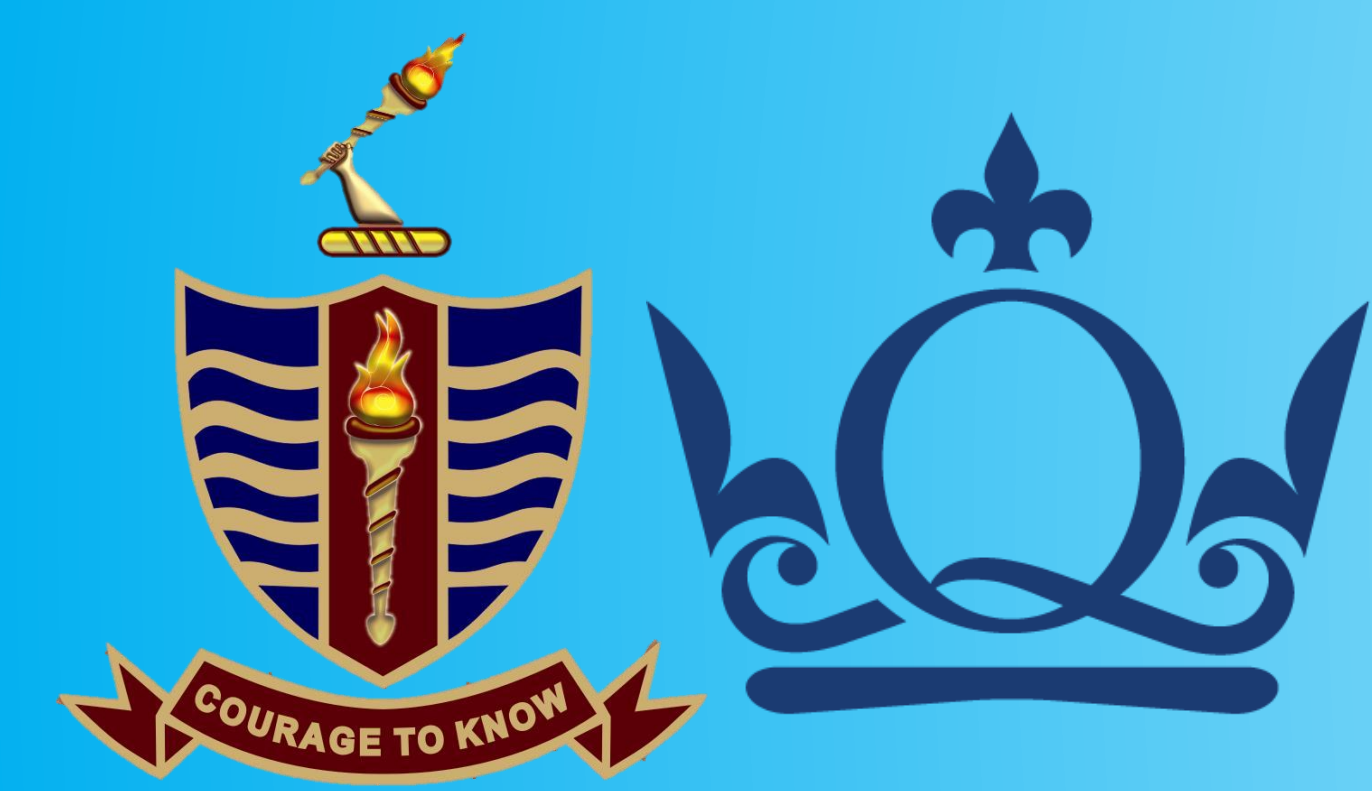
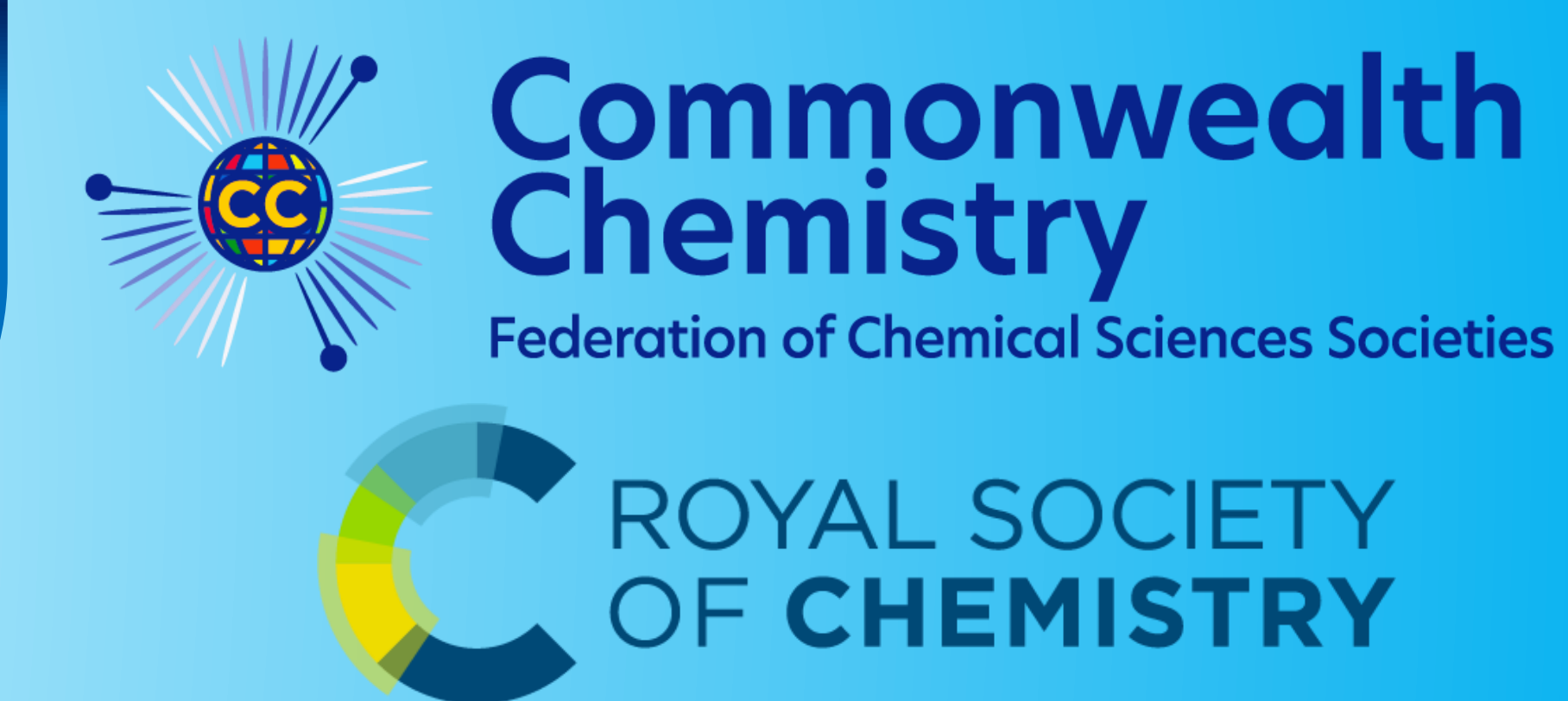




# Fused-Ring Nitrogen-rich Building Blocks to Design Non-fullerene Electron Acceptors for Organic Photovoltaics

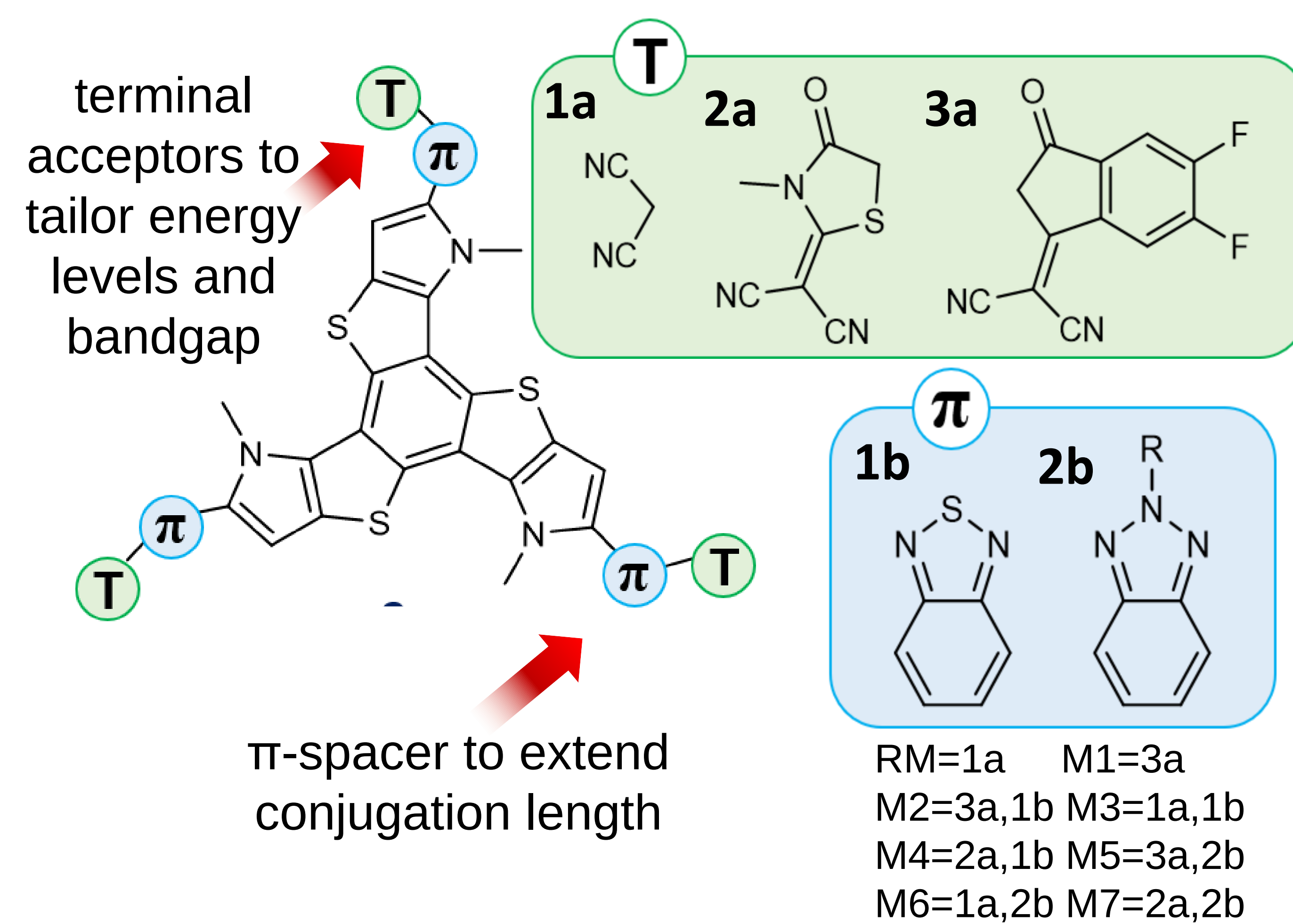


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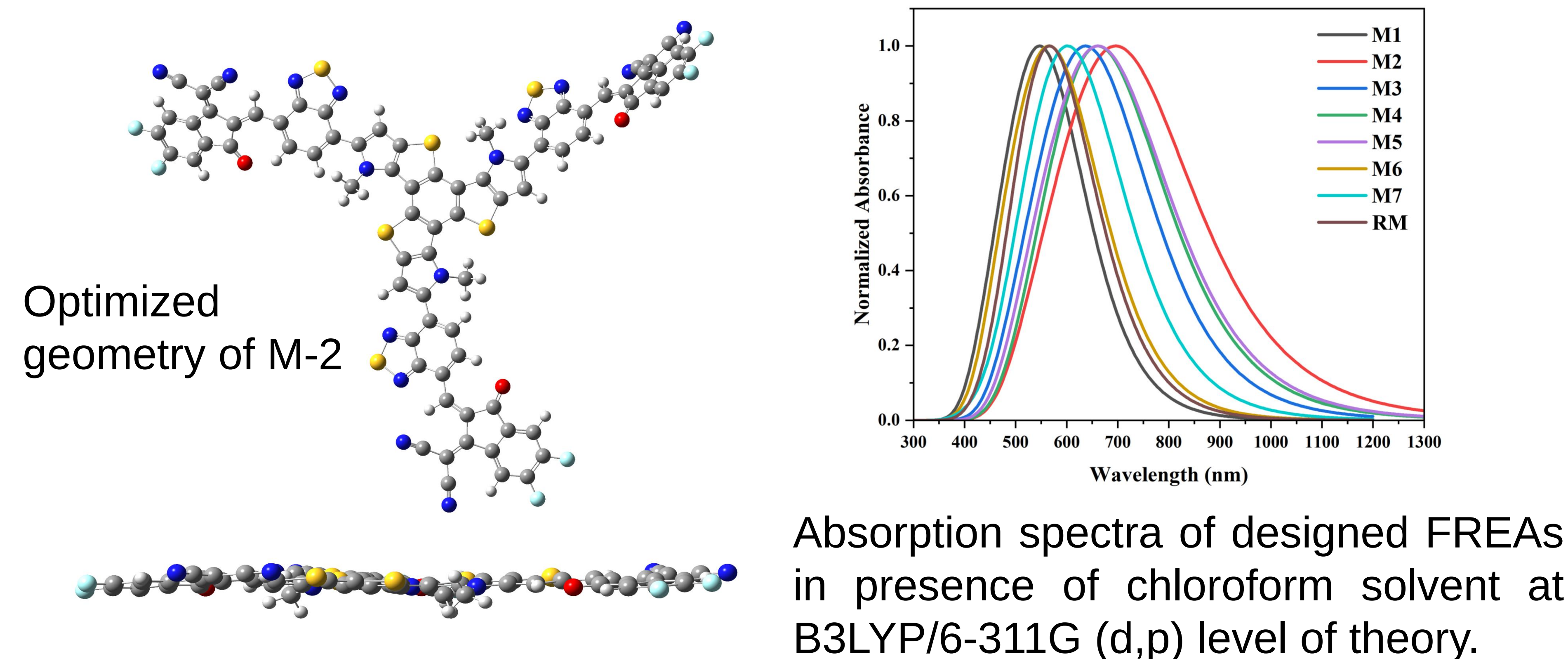
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## Introduction

Organic solar cells are amongst the most promising renewable energy conversion solutions due to their low-cost and flexibility. Fused-ring non-fullerene electron acceptors (FREAs) having well-connected  $\pi$ -conjugated framework enables higher electron charge transfer and electron mobilities, which has frequently exhibited champion PCE.<sup>1-3</sup> Herein, we introduce new multi-directional FREAs containing a Benzotrithienopyrrole central core connected to a  $\pi$ -bridge acceptor, either benzo[c][1,2,5] thiadiazole or benzo[d][1,2,3]triazole, and one of three terminal acceptors: 2-(5,6-difluoro-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile, malononitrile, or 2-(3-methyl-4-oxothiazolidin-2-ylidene)malononitrile as FREAs for organic electronics.

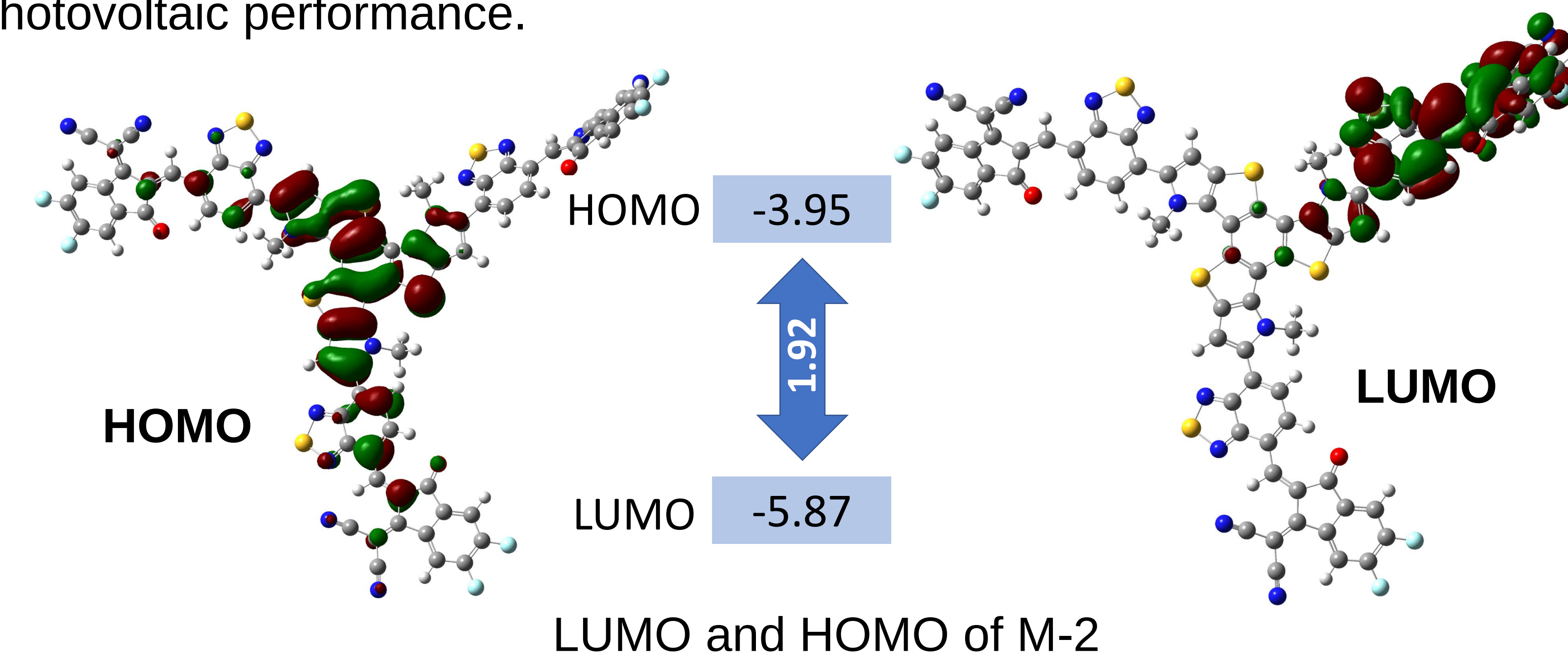


## Geometry and Spectral Analysis



## Frontier Molecular Orbitals

Computational studies performed on Gaussian 16, using DFT B3LYP/6-311g (d,p) basis set revealed the adjustable bandgap by using different combinations of bridging and terminal units thus allowing structure tunability for optimum photovoltaic performance.



Electricity for remote places



Building-integrated power solutions

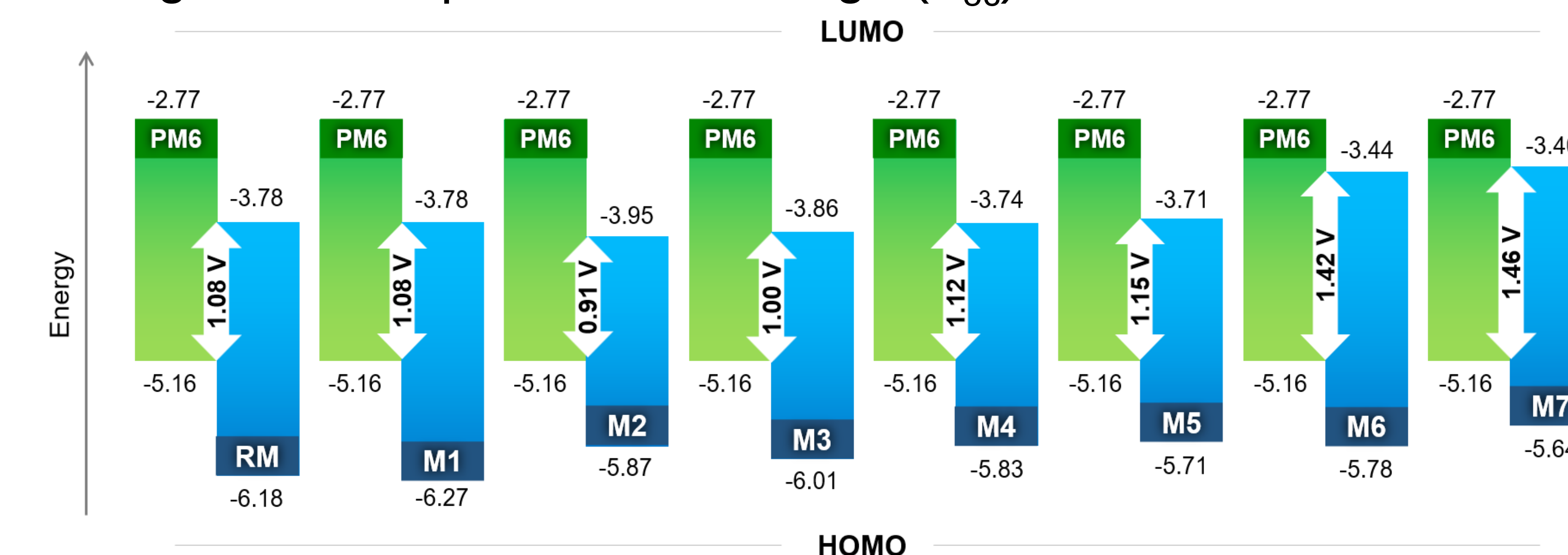


Light-weight and low-cost electronics



## Open Circuit Voltage

In this study, we employed a combination of the PM6 donor material with RM and newly proposed FREAs, M1-M7, to investigate their Open Circuit Voltage ( $V_{oc}$ ).



## References

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