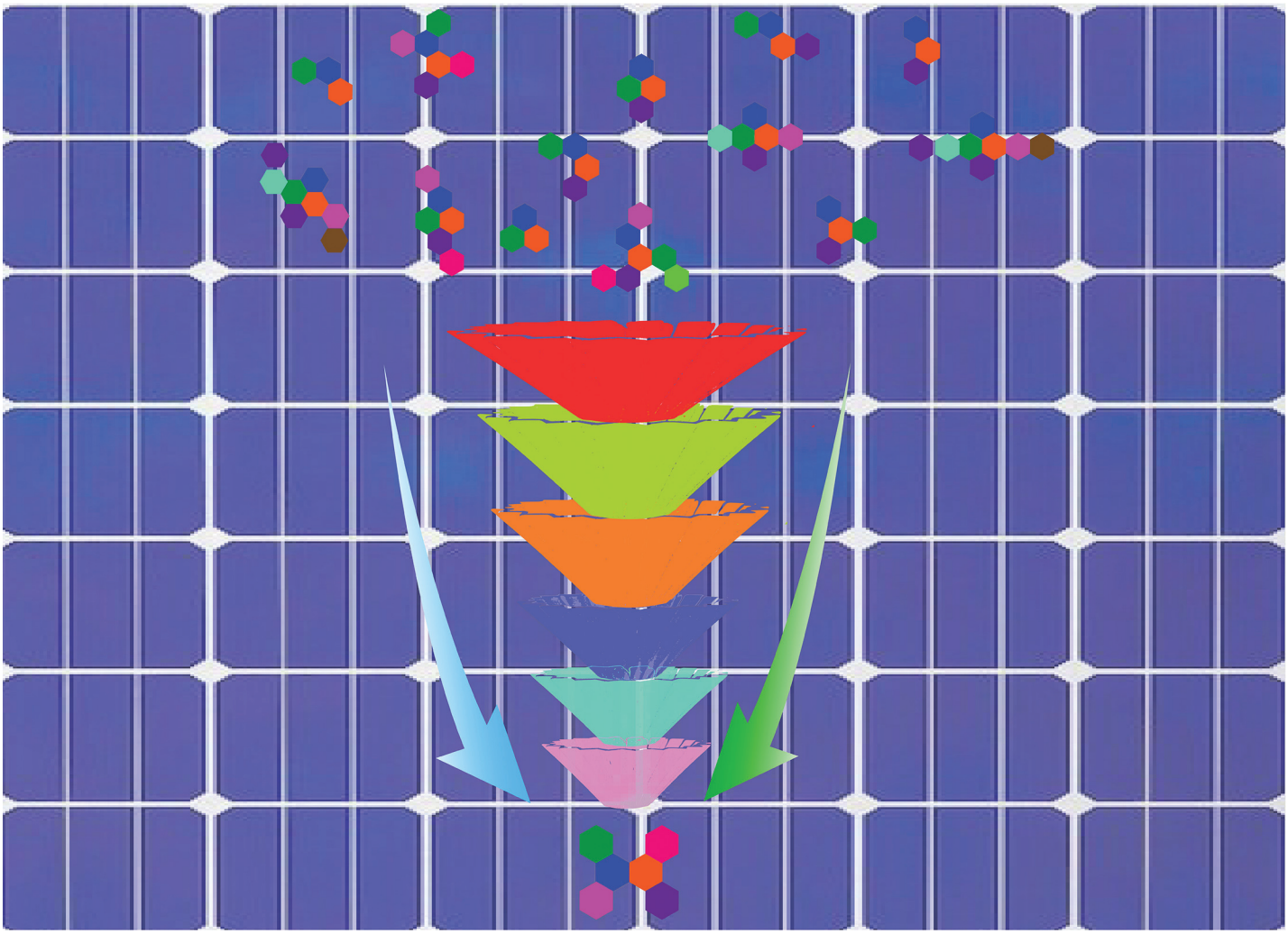

Showcasing collaborative research from Dr. Tanay Kundu, SRM Institute of Science & Technology and Dr. Amrita Pal's laboratory, Department of Chemistry, and Sathyabama Institute of Science and Technology, Chennai, India.

Six-fold screening unfolds optimized rylene diimides towards organic solar cells: a DFT perspective

Sunlight to sustainable electricity conversion requires effective screening of donor–acceptor materials with broadband absorption, electrical mobility and charge separation. Here, rylene diimides have been shortlisted as model acceptors in solar cells. The role of expanding the rylene core (pyromellitic to bisazulene); changing ring size (5-member and 6-member) and positions (2,3- *vs.* 1,8/9) of the diimide; changing diimide sidechain from alkyl to aryl, and twisting core-planarity of the rylene (pyrene to corannulene) reveals six-step screening that predicts the candidate with the highest electron mobility in the series.

Image reproduced by permission of Amrita Pal from *Dalton Trans.*, 2025, **54**, 8076.

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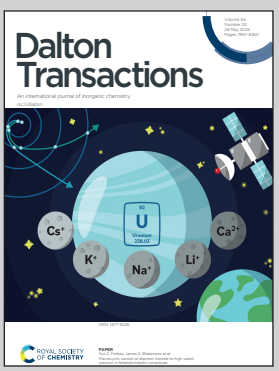

See Sri Vanaja, Tanay Kundu and Amrita Pal, *Dalton Trans.*, 2025, **54**, 8076.

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