

Poster Presentation
Inter-Disciplinary Explorations in Chemistry (I-DEC 2018)

Environment-Sensitive Tunable Emission through Intramolecular Charge Transfer in T and V-Shaped Donor-Acceptor-Donor Molecules

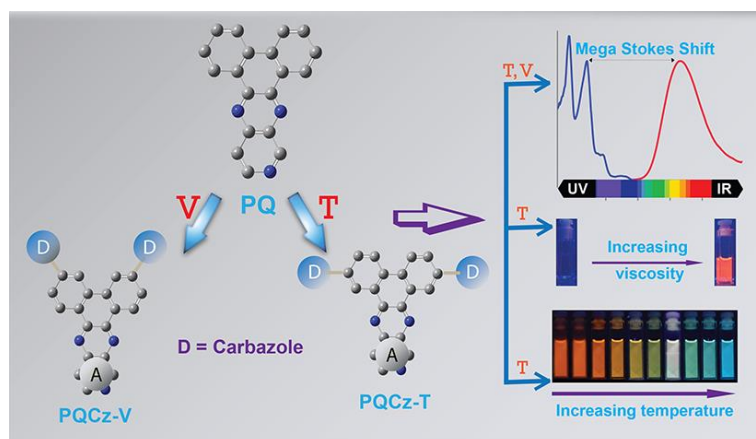
Bahadur Sk, Saurabh Khodia, Samarth Sharma, Abhijit Patra*

Department Chemistry, IISER Bhopal

Bhauri, Bhopal Bypass Road, Bhopal – 462066, Madhya Pradesh, INDIA

(E-mail: abhijit@iiserb.ac.in)

Organic push–pull chromophores, in which electron donor (D) and electron acceptor (A) units are connected through π -linkers have been extensively studied because of their rich photophysical properties and potential applications in optoelectronic materials and devices.¹ The most fundamental phenomenon governing the interesting optical properties of these molecules is intramolecular charge transfer (ICT) from the donor to the acceptor unit in the excited state. The molecular geometry has a profound impact on the ICT process. Often, ICT proceeds with drastic conformational changes in certain D–A molecules leading to the formation of a twisted intramolecular charge transfer (TICT) state. As the TICT emission is highly environment-sensitive and depends on the solvent polarity, viscosity and temperature of the medium, such fluorophores are potential candidates for designing optical sensors.²⁻³ We have designed a new class of donor–acceptor–donor (D–A–D) type molecules having a novel acceptor core of pyridoquinoxaline (PQ). The placing of electron donating carbazole (Cz) unit at 2,7 and 3,6-positions of phenanthrene analogue of PQ leads to T and V-shaped molecules (PQCz-T and PQCz-V). We have demonstrated that the facile conjugation across the entire molecule in the V-shaped molecule leads to the diminished charge transfer as compared to T-shaped molecule. As a result, PQCz-T exhibits a large Stokes shift, red emission in the solid state, remarkable viscosity and temperature-dependent tunable fluorescence including a thermally-induced single-component near white-light emission.⁴ Currently, we are exploring the intimate details of the charge transfer attributes in a series of D–A–D molecules.



Scheme: Schematic illustration of environment-sensitive tunable emission in T and V- shaped D-A-D based molecular materials

References and Notes:

1. Lippert, E.; Luder, W.; Boos, H., *Advances in Molecular Spectroscopy*, Pergamon: **1962**; pp 443-457.
2. Grabowski, Z. R.; Rotkiewicz, K.; Rettig, W., *Chem. Rev.* **2003**, *103*, 3899-4031.
3. Sasaki, S.; Drummen, G. P. C.; Konishi, G., *J. Mater. Chem. C* **2016**, *4*, 2731-2743.
4. Sk, B.; Khodia, S.; Patra, A., *Chem. Commun.* **2018**, *54*, 1786-1789.