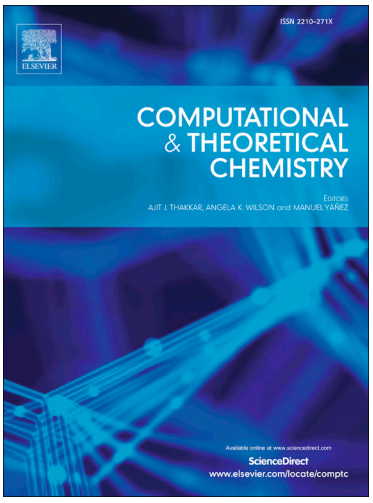

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G. Krishna Chaitanya, Avinash L. Puyad, K. Bhanuprakash

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The Extent of Charge Transfer: A Qualitative Computational Study on Electronic Transitions of Unsymmetrical Squarylium Dyes

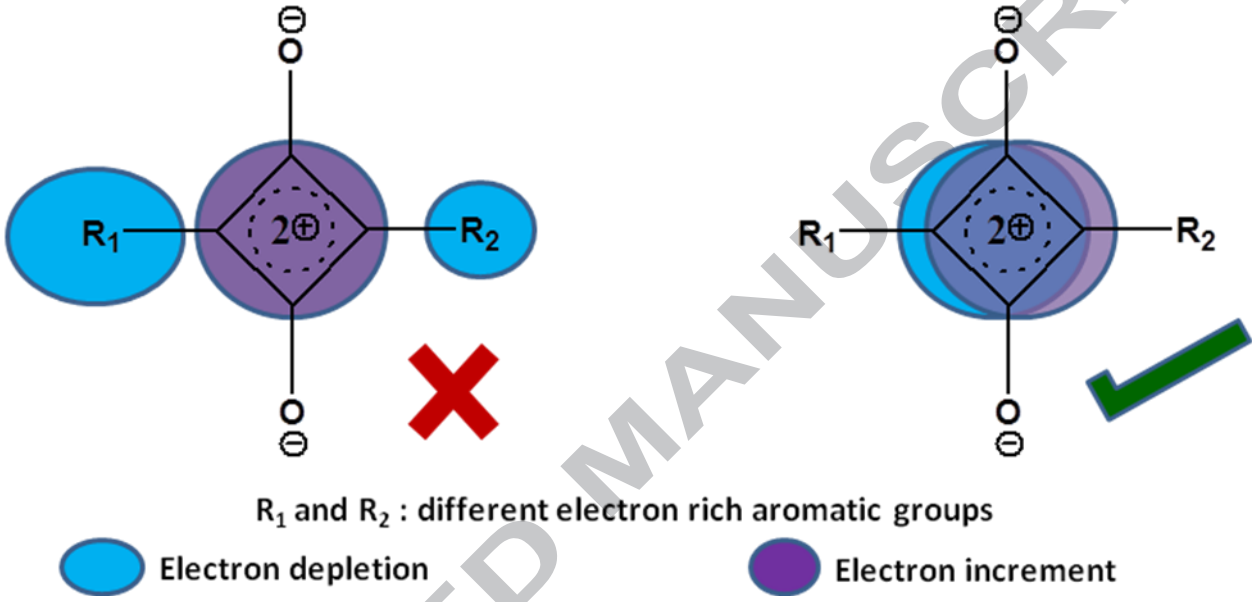
G. Krishna Chaitanya,[a,*] Avinash L. Puyad,[a] K. Bhanuprakash[b]

[a]*School of Chemical Sciences, S.R.T.M. University, Nanded-431 606, India.*

[b]*Inorganic Chemistry Division, Indian Institute of Chemical Technology, Hyderabad,India*

* corresponding author E-mail: krishnachaitanya.gunturu@gmail.com

Graphical Abstract



Highlights

- The impact of different electron rich aromatic substituent side groups attached to central SQ moiety is limited to structural effects.
- No significant charge transfer (CT) is seen in UNSQ derivatives during lowest energy absorption.
- Le Bahers's diagnosing indexes obtained with (TD)DFT and SAC-CI levels are almost similar though absorption maximum is different from both methodologies.
- No additional advantage of USQ when compared with symmetrical SQ analogs is found in terms of CT whereas only charge reorganization is seen in both the cases.

Abstract:

The nature of lowest energy electron transitions of unsymmetric squarylium (USQ) dyes has been studied through ab-initio and DFT methods with Le Bahers's diagnosing indexes. Soliton structure of atomic charge alternation and bond length alternation data indicates the