

MSDE

Molecular Systems Design & Engineering rsc.li/molecular-engineering

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

ISSN 2058-9689 CODEN MSDEBG 10(1) 1–82 (2025)



Cover

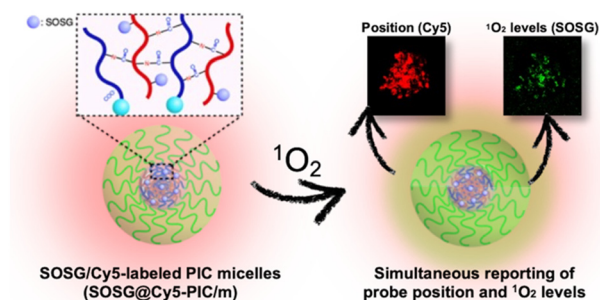
See Thi Vo et al.,
pp. 19–31.
Image reproduced by
permission of Thi Vo from
Mol. Syst. Des. Eng., 2025,
10, 19.

COMMUNICATIONS

7

Dual-labelled polymeric micelles for singlet oxygen reporting in biological systems

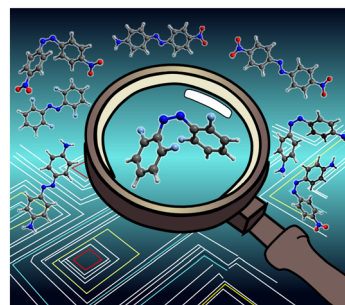
Yasuhiro Nakagawa, Hayato Laurence Mizuno, Yuta Ushimaru, Jumpei Norimatsu, Kazunori Igarashi, Keita Masuda, Madoka Takai, Yasutaka Anraku and Horacio Cabral*



13

Is DFT enough? Towards accurate high-throughput computational screening of azobenzenes for molecular solar thermal applications

Flavia Aleotti,* Lorenzo Soprani, Lucas F. Rodríguez-Almeida, Francesco Calcagno, Fabio Loprete, Ivan Rivalta, Silvia Orlandi, Elisabetta Canè, Marco Garavelli,* Irene Conti* and Luca Muccioli*



ChemComm

Uncover new possibilities with outstanding preliminary research

Original discoveries, fuelling
every step of scientific progress

rsc.li/chemcomm

**Fundamental questions
Elemental answers**

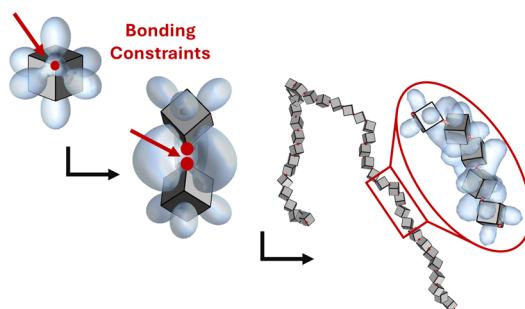


PAPERS

19

Elucidating the interplay between entropy-driven and patch-mediated bonding in directing nanoscale assemblies

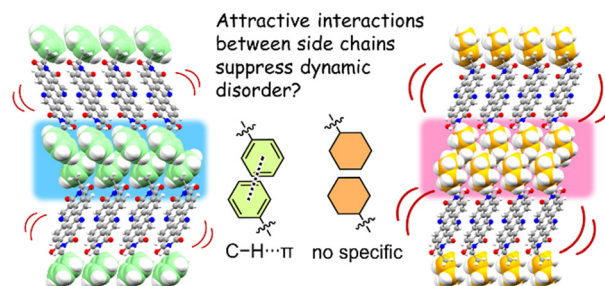
Kireeti Akkunuri, Xiangyu Zhang and Thi Vo*



32

Phenyl- versus cyclohexyl-terminated substituents: comparative study on aggregated structures and electron-transport properties in n-type organic semiconductors

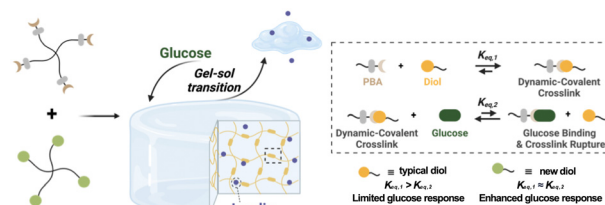
Shohei Kumagai,* Takeru Koguma, Yutaro Arai, Go Watanabe, Hiroyuki Ishii, Jun Takeya and Toshihiro Okamoto*



40

Enhanced glucose-responsivity of PBA-diol hydrogel networks by reducing crosslink affinity

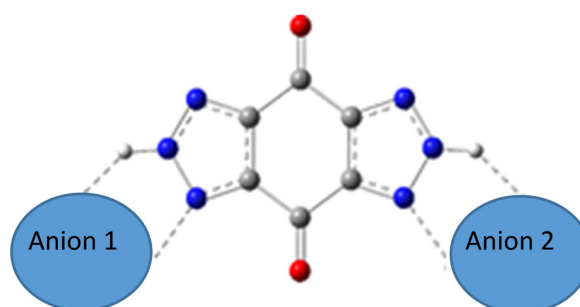
Sijie Xian, Yuanhui Xiang, Svenja Deichmann and Matthew J. Webber*

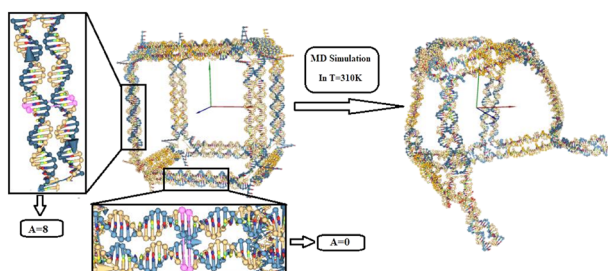


50

The structural, electronic and thermodynamic properties of the designed *p*-benzoquinone based dicationic ionic liquids: insight from DFT-GD3 and QTAIM

Hossein Roohi,* Sajedah Habibipour and Khatereh Ghauri





Wireframe DNA origami nanostructure with the controlled opening of edges

Maryam Mogheiseh and Reza Hasanzadeh Ghasemi*

