

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 8(10) 1223-1330 (2023)



Cover

See Scott Bobbitt, Jeffery A. Greathouse *et al.*, pp. 1257–1274. Image reproduced by permission of Scott Bobbitt from *Mol. Syst. Des. Eng.*, 2023, **8**, 1257. Artwork created by Daniel S. Thompson.



Inside cover

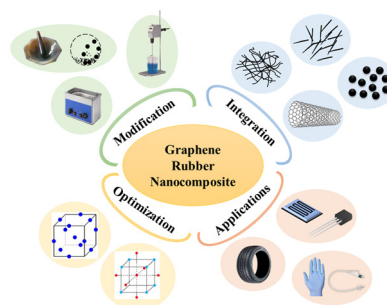
See Huaiyu Yang *et al.*, pp. 1275–1285. Image reproduced by permission of Huaiyu Yang from *Mol. Syst. Des. Eng.*, 2023, **8**, 1275.

REVIEW

1229

Graphene in rubber formulations: a comprehensive review and performance optimization insights

Y. L. Leong, H. N. Lim* and I. Ibrahim

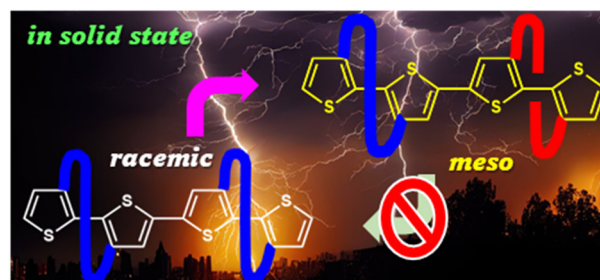


COMMUNICATION

1252

Studies on the stereochemical behaviors of a winding vine-shaped molecular wire of a bithiophene dimer with molecular asymmetry

Kohei Hosokawa, Kohei Tabuchi, Yuki Nakanishi, Kentaro Okano, Masaki Horie and Atsunori Mori*



Editorial Staff

Executive Editor

Maria Southall

Deputy Editor

Bianca Provost

Editorial Production Manager

Chris Goodall

Assistant Editors

Sean Browner, Molly Colgate, Paul Scott, Alison Winder

Editorial Assistant

Basita Javeed

Publishing Assistant

Allison Holloway

Publisher

Sam Keltie

For queries about submitted papers, please contact

Emily Skinner, Editorial Production Manager in the first instance.

E-mail: molecularengineering@rsc.org

For pre-submission queries please contact

Maria Southall, Executive Editor.

E-mail: molecularengineering-rsc@rsc.org

MSDE (electronic: ISSN 2058-9689) is published 12 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 0WF.

All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to the Royal Society of Chemistry Order Department, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK

Tel +44 (0)1223 432398; E-mail: orders@rsc.org

2023 Annual (electronic) subscription price: £2211; \$3649.

Customers in Canada will be subject to a surcharge to cover GST.

Customers in the EU subscribing to the electronic version only will be charged VAT.

If you take an institutional subscription to any Royal Society of Chemistry journal you are entitled to free, site-wide web access to that journal. You can arrange access via Internet Protocol (IP) address at www.rsc.org/ip

Customers should make payments by cheque in sterling payable on a UK clearing bank or in US dollars payable on a US clearing bank.

Whilst this material has been produced with all due care, the Royal Society of Chemistry cannot be held responsible or liable for its accuracy and completeness, nor for any consequences arising from any errors or the use of the information contained in this publication. The publication of advertisements does not constitute any endorsement by the Royal Society of Chemistry or Authors of any products advertised. The views and opinions advanced by contributors do not necessarily reflect those of the Royal Society of Chemistry which shall not be liable for any resulting loss or damage arising as a result of reliance upon this material. The Royal Society of Chemistry is a charity, registered in England and Wales, Number 207890, and a company incorporated in England by Royal Charter (Registered No. RC000524), registered office: Burlington House, Piccadilly, London W1J 0BA, UK, Telephone: +44 (0) 207 4378 6556.

Advertisement sales:

Tel +44 (0) 1223 432246; Fax +44 (0) 1223 426017;

E-mail: advertising@rsc.org

For marketing opportunities relating to this journal, contact marketing@rsc.org

MSDE

Molecular Systems Design & Engineering

rsc.li/molecular-engineering

Building and designing systems from the molecular level

Editorial Board

Editor-in-Chief

Claire S. Adjiman, Imperial College London, UK

Deputy Editor-in-Chief

Andrew Ferguson, University of Chicago

Associate Editors

Luke Connal, Australian National University, Australia

Robert Riggelman, University of Pennsylvania, USA

Members

Linda Broadbelt, Northwestern University, USA
LaShanda Korley, University of Delaware, USA

Yongye Liang, Southern University of Science and Technology, China

Anja Palmans, Eindhoven University of Technology, The Netherlands

Patrick Stayton, University of Washington, USA

Advisory Board

Alfredo Alexander-Katz, MIT, USA

Helena Azevedo, Queen Mary University of London, UK

Andre Bardow, ETH Zurich, Switzerland

Jeremy Baumberg, University of Cambridge, UK

Eva Blasco, Heidelberg University, Germany

Joao Cabral, Imperial College London, UK

Neil Champness, University of Nottingham, UK

Paulette Clancy, John Hopkins University, USA

Marc-Olivier Coppens, UCL, UK

Graeme Day, University of Southampton, UK

Andrew deMello, ETH Zurich, Switzerland

Juan de Pablo, University of Chicago, USA

Cecile Dreiss, Kings College London, UK

Thomas Epps III, University of Delaware, USA

Lei Fang, Texas A&M University, USA

C. Daniel Frisbie, University of Minnesota, USA

Xuefeng Guo, Peking University, China

Kristi Kiick, University of Delaware, USA

Raju Kumar Gupta, Indian Institute of Technology Kanpur, India

Sarah Heilshorn, Stanford University, USA

Arthi Jayaraman, University of Delaware, USA

Takashi Kato, University of Tokyo, Japan

Sang Ouk Kim, KAIST, Republic of Korea

Jodie Lutkenhaus, Texas A&M University, USA

Heidi Mansour, University of Arizona, USA

Bert Meijer, Eindhoven University of Technology, Netherlands

Takashi Nakanishi, NIMS, Japan

Ki Tae Nam, Seoul National University, Republic of Korea

Insup Noh, Seoul National University of Science & Technology, Republic of Korea

Mark A. Olson, Tianjin University, China

Ho Bum Park, Hanyang University, South Korea

Jon Parquette, Ohio State University, USA

Boaz Pokroy, Technion – Israel Institute of Technology, Israel

Jeffrey Rimer, University of Houston, USA

Shu Seki, Kyoto University, Japan

Randy Snurr, Northwestern University, USA

Brigitte Stadler, Aarhus University, Denmark

Doros Theodorou, National Technical University of Athens, Greece

Matthew Tirrell, University of Chicago, USA

Bernhardt L. Trout, MIT, USA

Raymond W. Y. Wong, Hong Kong Polytechnic University, Hong Kong

Jia Zhu, Nanjing University, China

Meifang Zhu, Donghua University, China

Information for Authors

Full details on how to submit material for publication in MSDE are given in the Instructions for Authors (available from <http://www.rsc.org/authors>). Submissions should be made via the journal's homepage: rsc.li/molecular-engineering. Submissions: The journal welcomes submissions of manuscripts for publication as Review Articles and Minireviews. Full Papers and Communications should describe original work of high quality and impact.

Additional details are available from the Editorial Office or

<http://www.rsc.org/authors>

Authors may reproduce/republish portions of their published contribution without seeking permission from the Royal Society of Chemistry, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation)–Reproduced by permission of the Royal Society of Chemistry.

This journal is © The Royal Society of Chemistry 2023.

Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

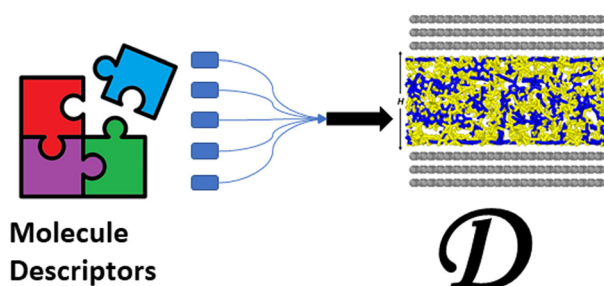
Registered charity number: 207890



1257

Machine learning predictions of diffusion in bulk and confined ionic liquids using simple descriptors

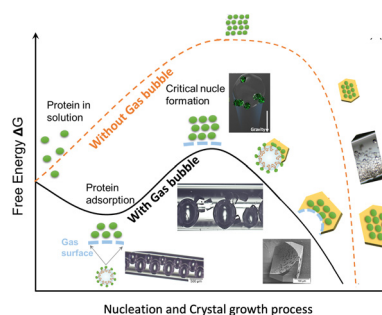
N. Scott Bobbitt,* Joshua P. Allers, Jacob A. Harvey, Derrick Poe, Jordyn D. Wemhoner, Jane Keth and Jeffery A. Greathouse*



1275

Protein crystallisation with gas microbubbles as soft template in a microfluidic device

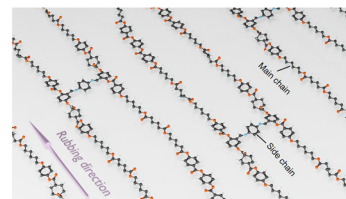
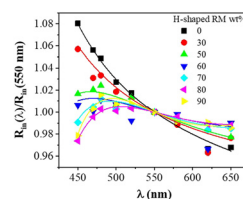
Wenqing Tian, Oladayo Ogunyinka, Charlie Oretti, H. C. Hemaka Bandulasena, Chris Rielly and Huaiyu Yang*



1286

Effect of intra-cyclohexane rings in H-shaped reactive molecules on the negative dispersion of optical retardation

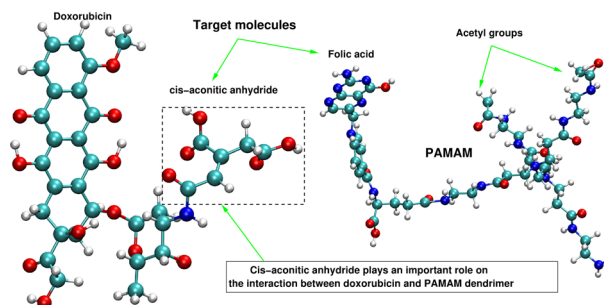
Hoai Thu Luong, Ja Won Kim, Jiyun Lee, Yi Young Kang, Yumi Cho, Jae-Won Ka,* Sang Kyu Kwak* and Ji-Hoon Lee*



1295

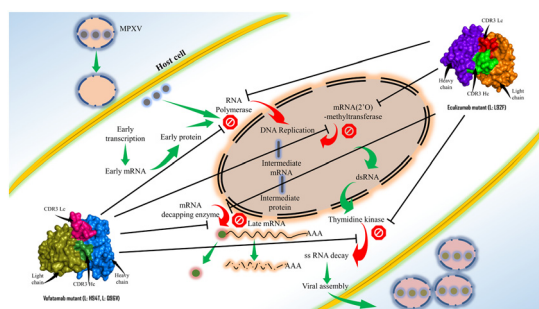
Describing the adsorption of doxorubicin on a PAMAM dendrimer by *ab initio* calculations

Handriela Hoff de Oliveira Sobrinho, Renato Eising and Ernesto Osvaldo Wrasse*



PAPERS

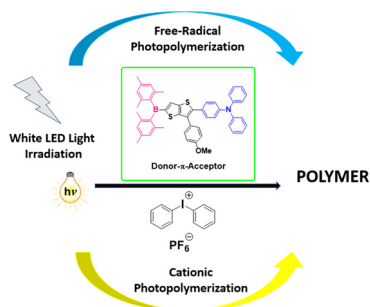
1301



Multifaceted mutational immunotherapeutic approach to design therapeutic mAbs to combat monkeypox disease *via* integrated screening algorithms and antibody engineering

Satyendra Singh, Abhishek Rao, Anshuman Mishra, Amit Mishra and Vijay Kumar Prajapati*

1319



Cationic and radical polymerization using a boron-thienothiophene-triphenylamine based D- π -A type photosensitizer under white LED irradiation

Ali Suerkan, Recep Isci,* Turan Ozturk and Yusuf Yagci*

CORRECTION

1327

Correction: Describing the adsorption of doxorubicin on a PAMAM dendrimer by *ab initio* calculations

Handriela Hoff de Oliveira Sobrinho, Renato Eising and Ernesto Osvaldo Wrasse*

