

IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 27(26) 13757–14156 (2025)



Cover

See Masahiro Yoshizawa-Fujita *et al.*, pp. 13826–13835. Image reproduced by permission of Masahiro Yoshizawa-Fujita from *Phys. Chem. Chem. Phys.*, 2025, 27, 13826.



Inside cover

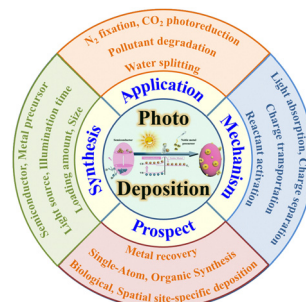
See Georgios Katsoukis, Jeffrey A. Kelber *et al.*, pp. 13836–13844. Image reproduced by permission of Georgios Katsoukis from *Phys. Chem. Chem. Phys.*, 2025, 27, 13836.

REVIEWS

13770

Synthesis, photocatalytic applications and future prospects of noble metal-modified semiconductors fabricated *via* photodeposition

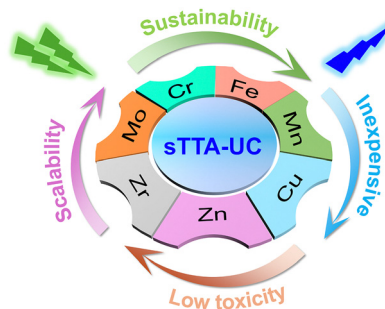
Faqi Zhan,* Jiahao Qi, Ruixin Li, Haiyan Zhao, Yisi Liu and Peiqing La*



13793

Photon upconversion sensitized by earth-abundant transition metal complexes

Pengyue Jin and Cui Wang*



RSC Applied Interfaces

GOLD
OPEN
ACCESS

Interfacial and surface research with an applied focus

Interdisciplinary and open access



rsc.li/RSCApplInter

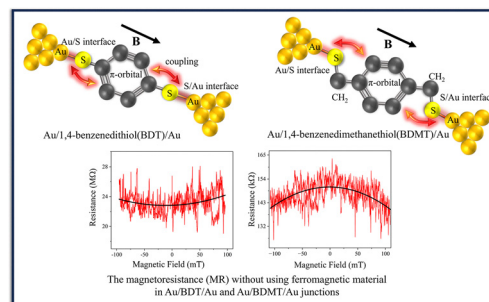
Fundamental questions
Elemental answers

COMMUNICATIONS

13812

Magnetoresistance in Au/1,4-benzene-dithiol/Au and Au/1,4-benzene-dimethanethiol/Au single-molecule junctions

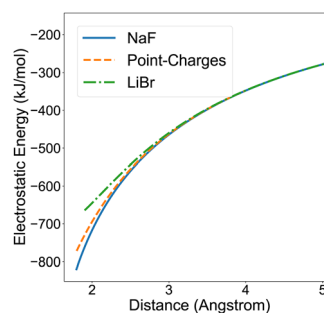
Rachmat Andika, Grace Gita Redhyka, Ryo Yamada* and Hirokazu Tada*



13817

Point + Gaussian charge model for electrostatic interactions derived by machine learning

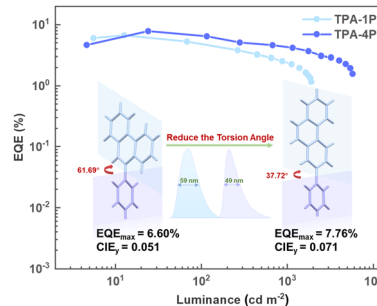
David van der Spoel* and A. Najla Hosseini



13821

Manipulating excited states of non-doped deep blue emitter by adjusting the intramolecular torsion angle

Ling Lin, Mingke Li, Yulong Li, Youran Lin, Yu Huang, Yue Yu,* Lei Ying and Yuguang Ma*

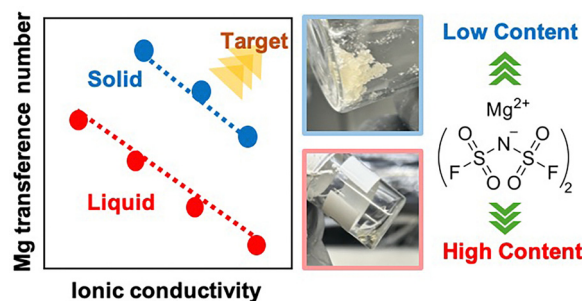


RESEARCH PAPERS

13826

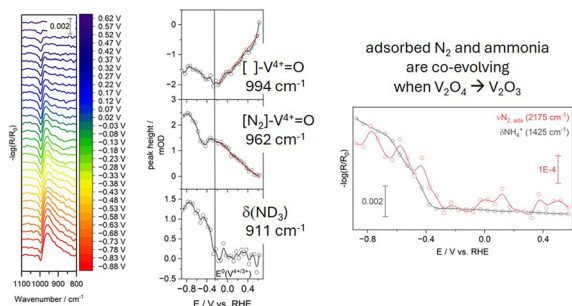
Enhanced ion-transport characteristics of pyrrolidinium-based electrolytes with $\text{Mg}(\text{FSA})_2$

Yoshifumi Hirotsu, Mizuki Kimura, Shinkoh Nanbu, Yuko Takeoka, Masahiro Rikukawa and Masahiro Yoshizawa-Fujita*



RESEARCH PAPERS

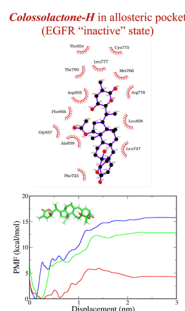
13836



Correlating reductive vanadium oxide transformations with electrochemical N₂ activation and ammonia formation

Kabir Balogun, Qasim Adesope, Stella Amagbor, Agbara Tochi, Adam Vass, Guido Mul, Christoph Baeumer, Georgios Katsoukis* and Jeffry A. Kelber*

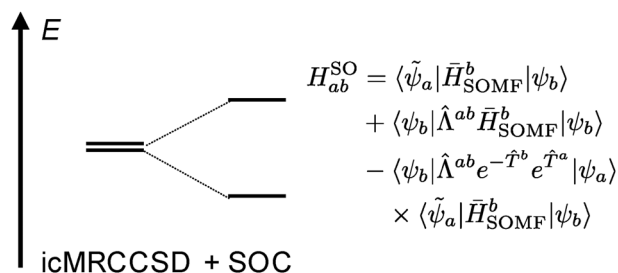
13845



Molecular dynamics simulations reveal a strong binding capacity of colossolactone H to the EGFR inactive conformation

Duc Toan Truong, Kiet Ho, Chinh Tam Thai, Dung Do Thi Mai, Nguyen Minh Tam, Viet Bac T. Phung and Minh Tho Nguyen*

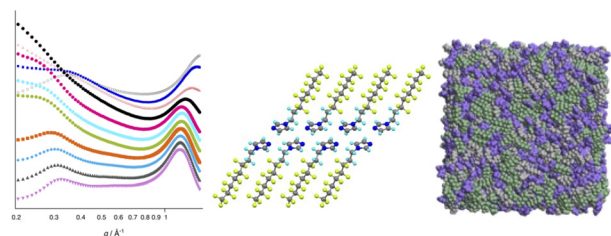
13861



Treatment of spin-orbit coupling with internally contracted multireference coupled cluster theory

Andreas Köhn* and Julia Netz

13870



To mix or not to mix: charge and polarity effects on alkyl/fluoroalkyl compound miscibility

Joshua Lai, Evelyn F. Gladden-Bennett, Karina Shimizu,* Naomi S. Elstone, Theo F. N. Tanner, Bruno Demé, Adrian C. Whitwood, Seishi Shimizu, Jose N. Canongia Lopes, John M. Slattery* and Duncan W. Bruce*

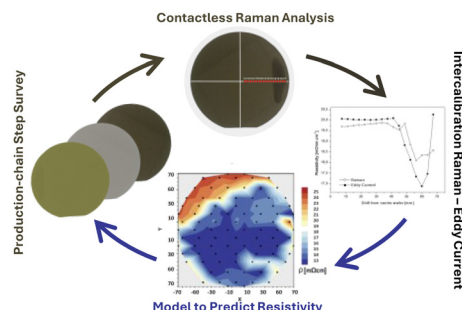


RESEARCH PAPERS

13884

Resistivity mapping of SiC wafers by quantified Raman spectroscopy

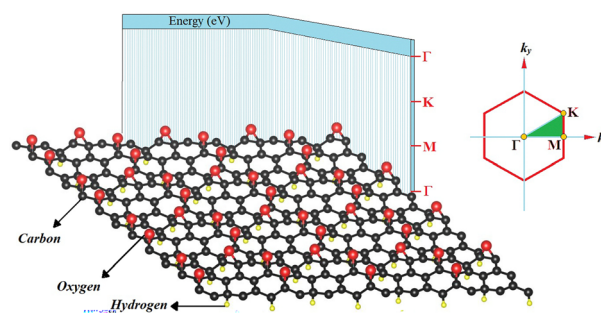
Elisa Calà, Simone Cerruti, Cristina Sanna, Marco Maffè, Wen Chin Hsu, Man Hsuan Lin, Luciano Ramello and Giorgio Gatti*



13893

Dual-functionalization of graphene: exploring flat bands and optical behavior

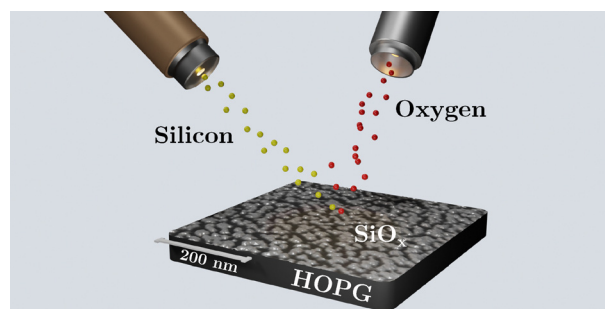
Nasim Hassani,* Ayoub Esmailpour, Mehdi Neek-Amal* and François M. Peeters



13906

Silicon oxide nanoparticles grown on graphite by co-deposition of the atomic constituents

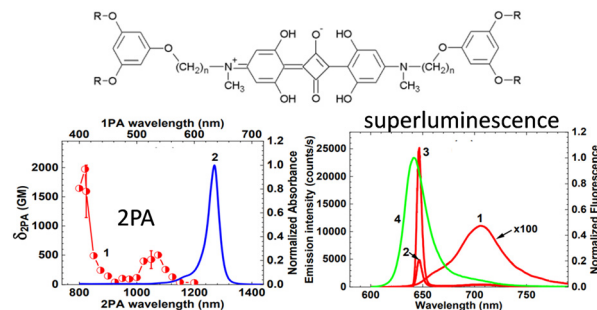
Steffen Friis Holleufer,* Alfred T. Hopkinson, Duncan S. Sutherland, Zheshen Li, Jeppe V. Lauritsen, Liv Hornekaer and Andrew Cassidy*



13917

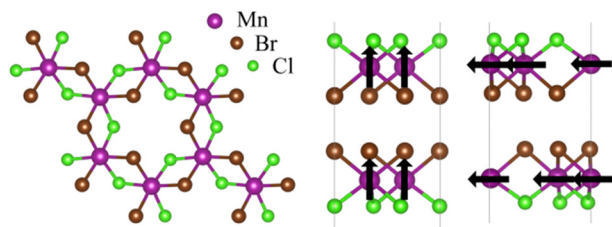
Nonlinear optical spectroscopy of new squaraine derivatives with high potential for multidisciplinary applications

George V. Klishevich, Volodymyr O. Hryn, Anton O. Kostetskyi, Iaroslav B. Kuziv, Igor Ya. Dubey, Yuri P. Piryatinski, Nataliia V. Bashmakova, Andriy M. Dmytruk, Viktor M. Kadan, Ivan V. Blonskyi and Mykhailo V. Bondar*



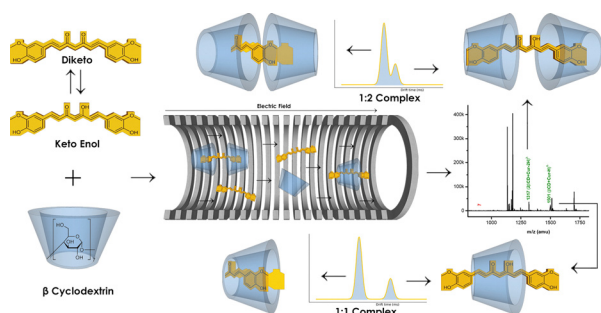
RESEARCH PAPERS

13929

Stacking-controlled magnetic anisotropy switching in bilayer Janus $\text{Mn}_2\text{Cl}_3\text{Br}_3$

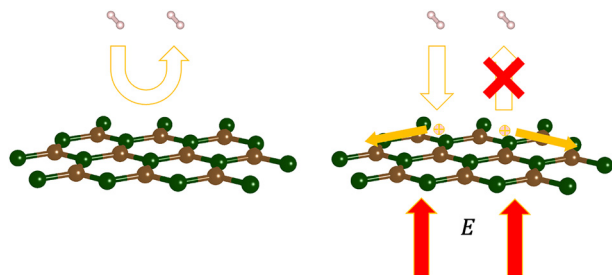
Yanle Liang, Heng Gao,* Hui Zhang,* Musen Li, Chang Liu, Zhaohe Gao, Cheng Tang and Wei Ren*

13939

Encapsulation effects on the structure and tautomeric distribution of curcumin in the β -cyclodextrin cavity: an ion mobility study

Megha Agarwal, Piyali Chatterjee and Tapas Chakraborty*

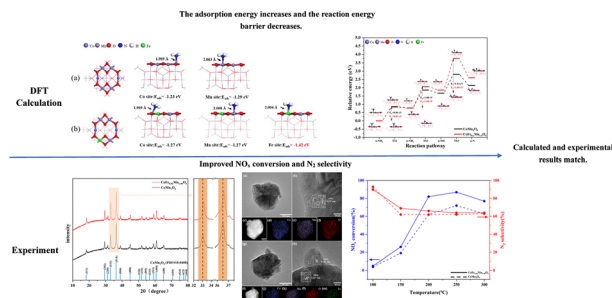
13952



Enabling hydrogen chemisorption on charged graphene

Patrick T. Shea, Andrew J. E. Rowberg and Brandon C. Wood*

13961

A combined DFT calculation and experimental study of the mechanism of the SCR of NO_x by NH_3 over Fe-doped CoMn_2O_4

Yulong Deng, Jiacheng Zheng, Wenting Chen, Xu Wang, Chengliao Deng, Xiaoming Cai, Jinming Cai and Honglin Tan*

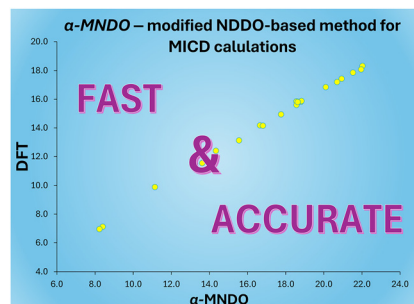


RESEARCH PAPERS

13976

Magnetically induced current density: a semiempirical approach

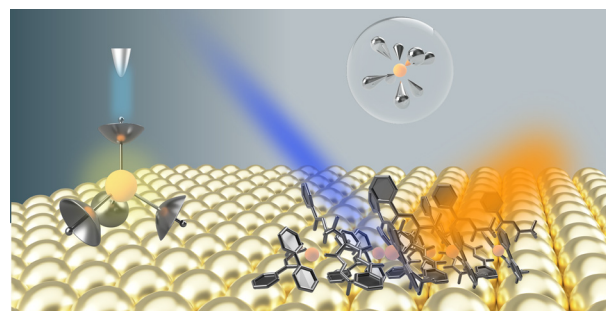
Slavko Radenković* and Slađana Đorđević



13984

Photoluminescence and self-assembly of three different Eu complexes

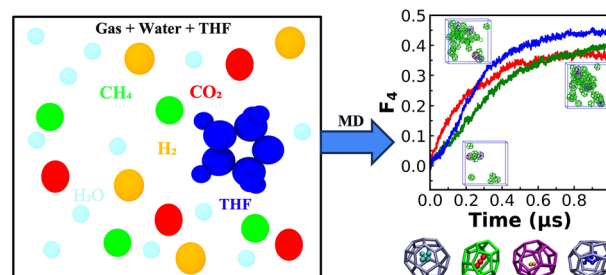
Adrian Ebert,* Lukas Gerhard, Julia Feye, Senthil Kumar Kuppusamy, Barbora Brachnakova, Mario Ruben, Peter W. Roesky and Wulf Wulfhekel



13991

Molecular dynamics insights into tetrahydrofuran-assisted formation of CH₄, CO₂, and H₂ gas hydrates

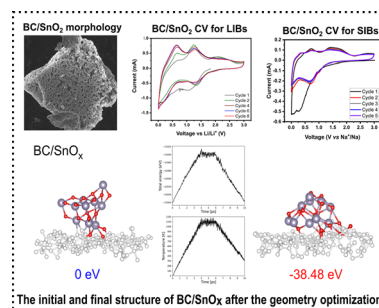
Ramkhelavan Kanaujiya, Atanu K. Metya,* Nilesh Choudhary, Rajnish Kumar and Tarak K Patra*

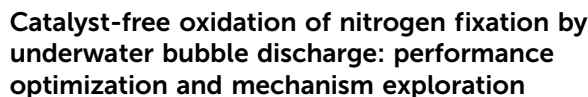


14000

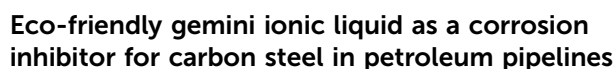
Biomass-derived macroporous carbon–tin oxide composites as stable and high-capacity anodes for lithium-ion and sodium-ion batteries: experimental study and GFN1-xTB calculations

Glaydson Simoes dos Reis,* Chandrasekar M Subramaniam, Alejandro Grimm, Mahiar Max Hamed, Palanivel Molaiyan, Flaviano Garcia-Alvarado, Ulla Lassi, Jakub Goclon and Shaikhshavali Petnikota





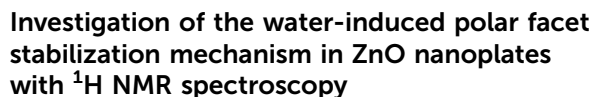
14029



14042



14054



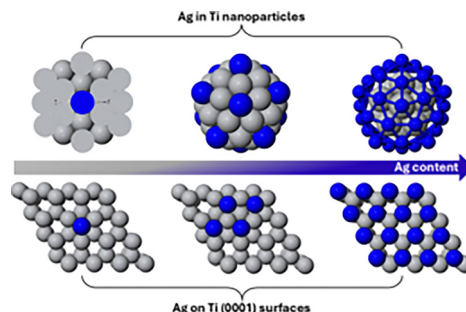
Benteng Song,* Qin Zhu and Ling-Hai Xie

RESEARCH PAPERS

14060

An *ab initio* study of silver–titanium interfaces in gas-phase and surface-supported clusters

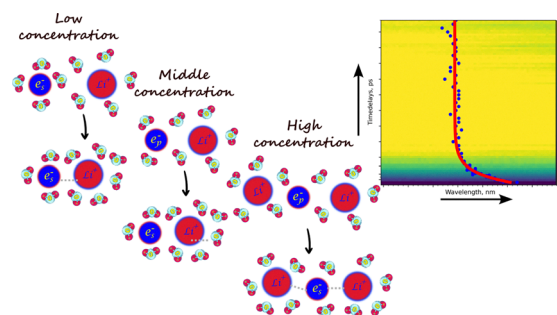
El yakout El koraychy* and Riccardo Ferrando*



14070

Solvation dynamics of electron–metal cation contact pairs in LiCl aqueous solutions

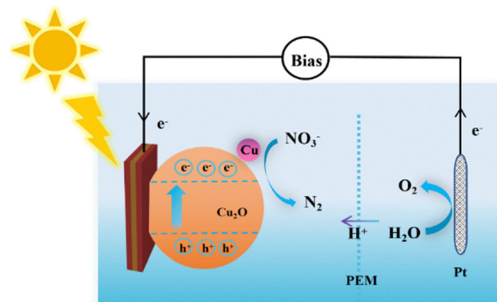
Denis Dobrovolskii, Mehran Mostafavi and Sergey A. Denisov*



14075

Photoelectrocatalytic reduction of nitrate to nitrogen gas by Cu₂O nanorod arrays on Cu foams with high stability

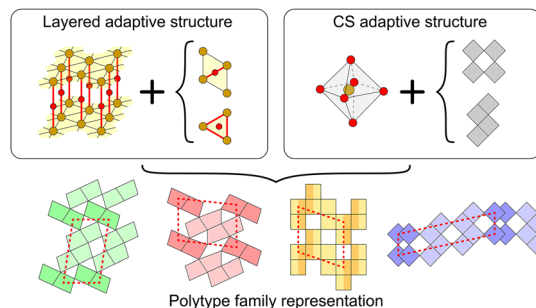
Wei Liu, Bin Huang, Peng Chen, Dongran Wang, Pengxiang Wang, Chuhong Zhu,* Zhulin Huang,* Haibin Tang* and Guowen Meng



14082

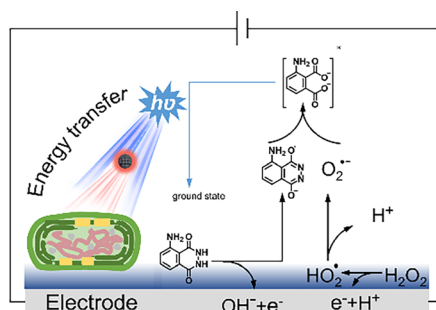
Polytype family representations of octahedrally coordinated adaptive structures in Ta₂O₅: energetic and dynamic stability from first principles

Dohyun Kim, Kun Hee Ye, Taeyoung Jeong, Seungjae Yoon, Yunjae Kim, Cheol Seong Hwang* and Jung-Hae Choi*



RESEARCH PAPERS

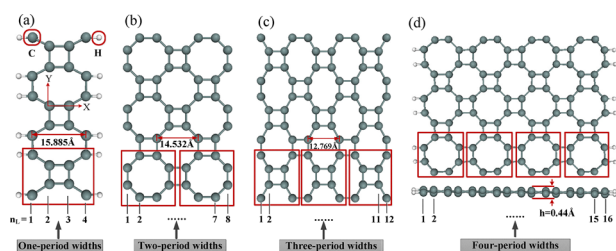
14095



Electrochemiluminescence and conjugated polymer-based photosynthesis system for regulating the photoreaction of a cyanobacterium

Kai Ma, Xiukun Zhang, Pengfei Wang, Chongyu Liang, Meiting Yi, Xiaoming Sun* and Zenghao Wang*

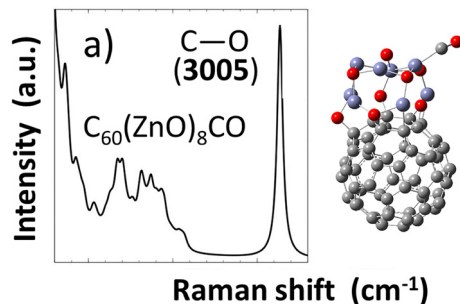
14100



Electronic band gap engineering of silicene allotropes: configuration-edge hydrogenation synergistic effect

Ya Liu, Lijun Wu* and Linhan He

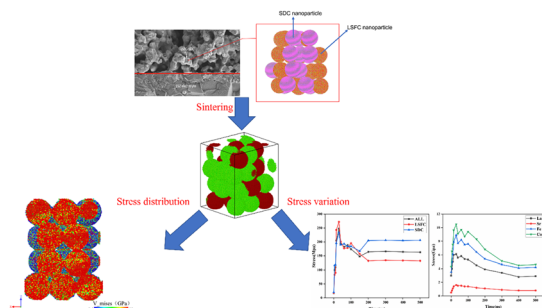
14113



Fullerene-enhanced Raman scattering: ZnO-covered C₆₀ as ultrasensitive CO gas sensor

A. Zamudio-Ojeda, S. J. Guevara-Martínez, J. G. Rodríguez-Zavala and R. A. Guirado-López*

14128



An all-atom molecular dynamics-based method for evaluating particle-level stress and diffusion of sintering La_{0.9}Sr_{0.1}Fe_{0.9}Co_{0.1}O_{3-δ}-Sm_{0.2}Ce_{0.8}O_{1.9} electrodes

Qijie Hang, Liusheng Xiao, Chenxia Wang, Tao Deng, Houxin Chi, Ding Rong Ou and Jinliang Yuan*



14143

Enhancement mechanism of electron–phonon coupling in XB_3 ($X = K$ and Rb) compounds with Kagome lattice

Xinwei Wang, Bohan Cao, Cheng Xing, Xiaoxuan Zhang, Haobo Li, Defang Duan,* Liang Li* and Fubo Tian*

