

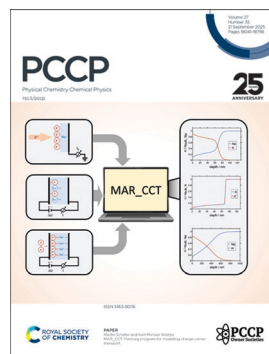
IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 27(35) 18041–18798 (2025)



Cover

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Inside cover

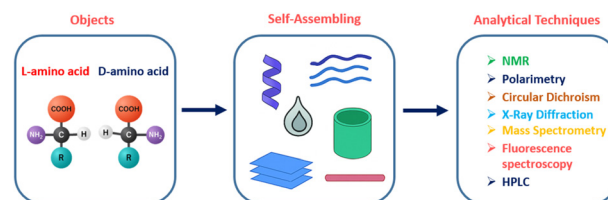
See Martin Schäfer and Karl-Michael Weitzel, pp. 18128–18140. Image reproduced by permission of Karl-Michael Weitzel from *Phys. Chem. Chem. Phys.*, 2025, 27, 18128.

TUTORIAL REVIEW

18062

Importance of chirality in the self-organizing peptides – from single molecules to functional supramolecular structures

Agata Chotera-Ouda, Katarzyna Trzeciak and Marek J. Potrzebowski*

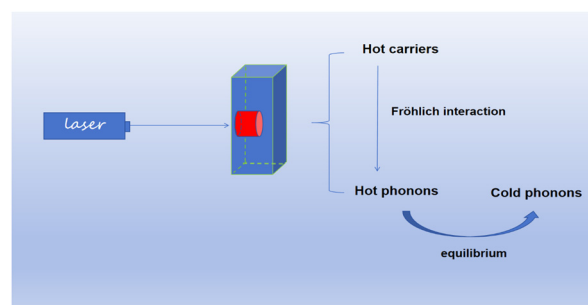


PERSPECTIVE

18093

Hot carriers and hot phonons in MAPbI₃ under pulsed excitation

Shuan Zhou, Chen-Guang Huang and Chen-Wu Wu*



Environmental Science: Atmospheres

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Fundamental questions
Elemental answers

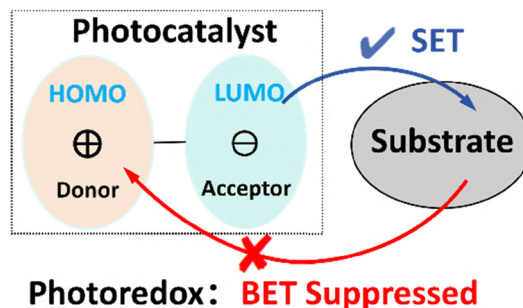


COMMUNICATIONS

18107

Intramolecular charge transfer state to suppress back electron transfer for singlet photoredox catalysis

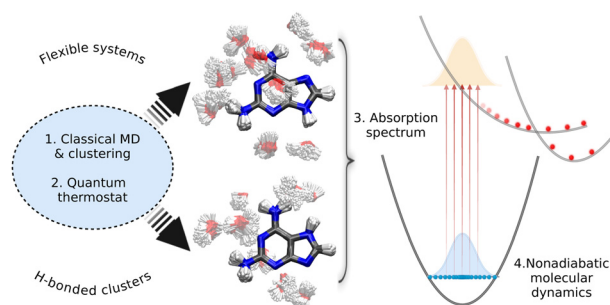
Yulong Ding and Shuming Bai*



18112

Investigating photodynamics of nucleobase–water systems

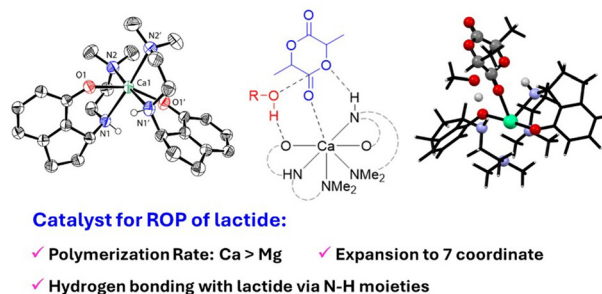
Haseena Sheik, Luca Grisanti, Tea Ostojić, Chaiyaporn Lakmuang, Barbara Rossi and Antonio Prlj*



18116

Homoleptic magnesium and calcium complexes supported by constrained reduced Schiff base ligand for lactide polymerisation: DFT analysis of lactide/ligand interactions

Trinity Quek, Thonthun Saeteaw, Tanyawan Pongpanit, Supawadee Namuangruk* and Khamphee Phomphrai*

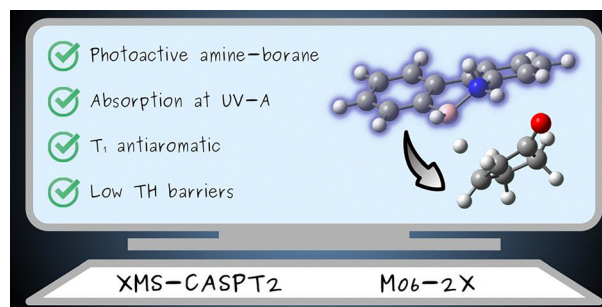


RESEARCH PAPERS

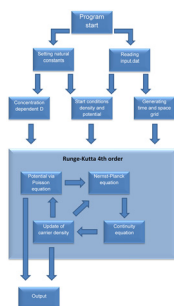
18121

Excited-state antiaromaticity relief in photoactive amine–boranes promotes transfer hydrogenation to electron-poor olefins

Enrique M. Arpa



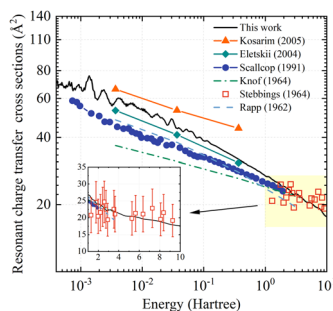
18128



MAR_CCT: Marburg program for modelling charge carrier transport

Martin Schäfer* and Karl-Michael Weitzel*

18141



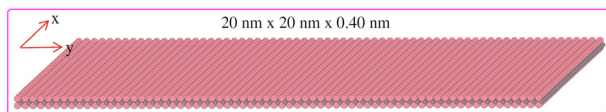
Resonance charge exchange and collision integrals for $O(^3P)-O^+(^4S)$ and $O(^1D)-O^+(^4S)$ interactions

Zi Ding and Linhua Liu*

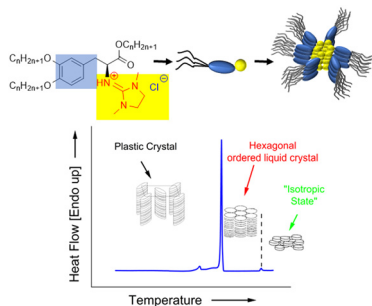
18152

Field-tunable skyrmion phases in monolayer MXene for spintronic applications

Junais Habeeb Mokkath*



18162



Molecular mobility and electrical conductivity of amino acid-based (DOPA) ionic liquid crystals in the bulk state and nanoconfinement

Mohamed A. Kolmangadi, Aileen R. Raab, Paulina Szymoniak, Zhuoqing Li, Patrick Huber, Sabine Laschat and Andreas Schönhals*

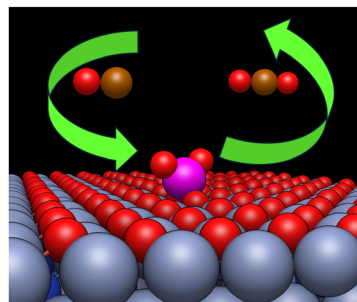


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18179

Single atom catalysts on the Cr_2NO_2 MXene for CO oxidation

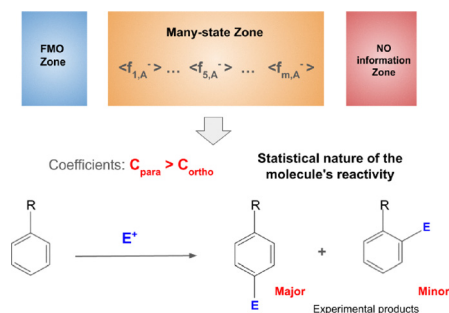
María Guadalupe Moreno-Armenta,*
Rodrigo Ponce-Perez, Francesc Viñes* and
Lourdes Mestres



18188

A statistical theory of reactivity based on molecular orbitals participation and its application to organic reactions

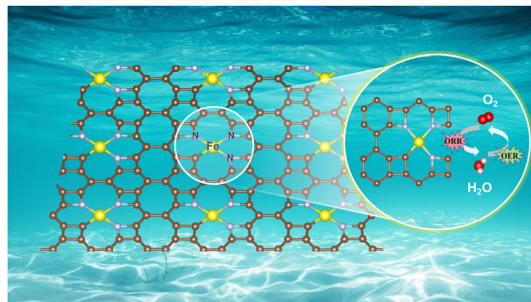
Javier Oller,* Paul Geerlings, Frank De Proft and
Pablo Jaque



18206

The regulation of the bifunctional electrocatalytic activity of transition metal atoms embedded in a biphenylene network by the asymmetric nitrogen coordination environment

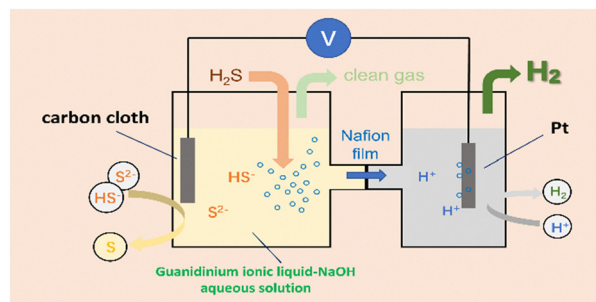
Lijia Luo, Zhengqin Zhao and Hui Wang*



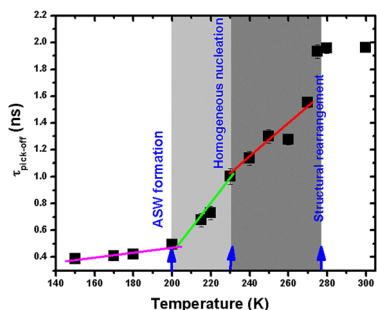
18214

Efficient capture and conversion of H_2S into H_2 and sulfur in guanidinium ionic liquid–NaOH aqueous solution

Qianqian Peng, Chengxuan Zhou, Shucan Qin,
Jinbiao Liang, Shengyun Xu, Jiaming Mao,
Jianming Shi, Yanrong Liu* and Yunqian Ma*



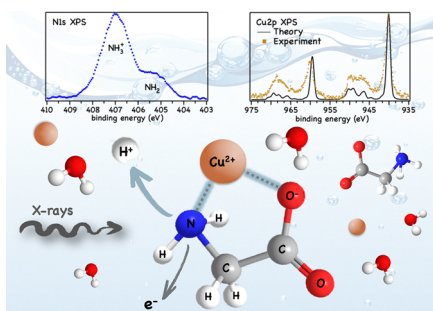
18222



Amorphous solid water prevails inside the spherical nanopores of the MIL-101(Cr) framework below 200 K: PALS, XRD and BDS studies

Vivek Sudhir, Debarati Das, Pranav Utpalla, Siddhartha Kolay, Manvendra Narayan Singh and Dhanadeep Dutta*

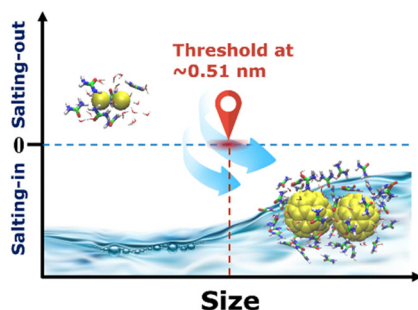
18234



Revealing ligand deprotonation and speciation pathways in Cu(II)–glycine aqueous solutions via liquid-jet X-ray photoelectron spectroscopy supported by *ab initio* calculations

D. Céolin, T. Saisopa,* Y. Rattanachai, S. Tangsukworakhun, W. Pokapanich, P. Songsirittigul, C. Songsirittigul, K. Klaiphet, J. Palaudoux, C. Nicolas and S. Carniato

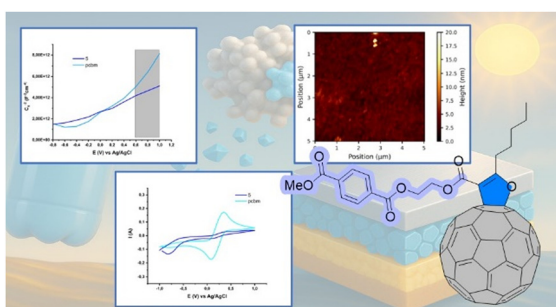
18248



Size-dependent desolvation of hydrophobic nanoparticles in aqueous osmolytes

Bing Fang, Guochao Sun, Yuanyuan Qu, Yong-Qiang Li, Xiangdong Liu, Yanmei Yang* and Weifeng Li*

18256



Early-stage analysis of PET – fullerene derivatives for electron transport in photovoltaics

Milica Đapović, Katarina Cvetanović, Vojislava Pošić, Vladislav Jovanov, Marko V. Bošković, Christos Polyzoidis, Nikolaos Tzoganakis, Konstantinos Rogdakis, Emmanuel Kymakis, Veselin Maslak* and Aleksandra Mitrović*

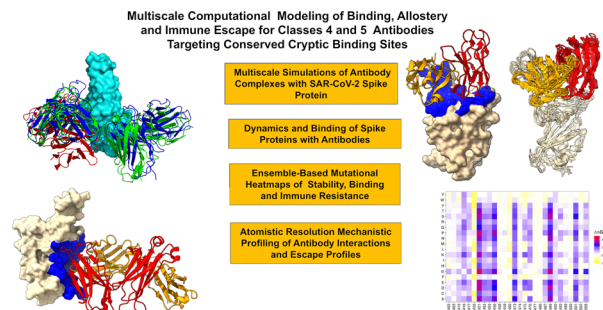


RESEARCH PAPERS

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Dynamic mutational profiling of binding interactions and allosteric networks in conformational ensembles of the SARS-CoV-2 spike protein complexes with classes of antibodies targeting cryptic binding sites: confluence of binding and allostery determines molecular mechanisms and hotspots of immune escape

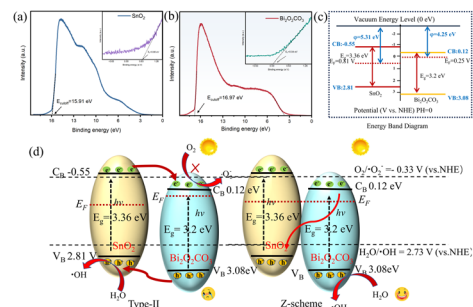
Mohammed Alshahrani, Vedant Parikh, Brandon Foley and Gennady Verkhivker*



18288

A pine cone-like $\text{SnO}_2/\text{Bi}_2\text{O}_2\text{CO}_3$ Z-scheme heterojunction photocatalyst enhances the photocatalytic degradation of tetracycline

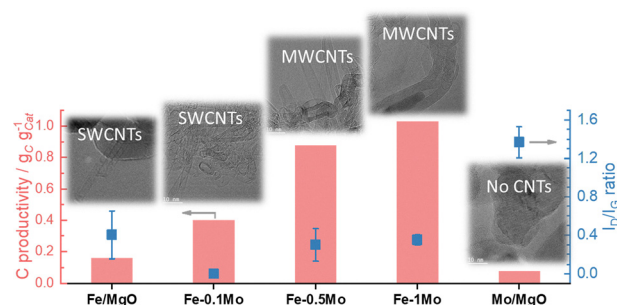
Xinyu Zheng, Shoufeng Zhang, Chen Liang, Peng Zhang, Jielu Yu,* Che Zhang* and Peng Gao*



18302

Tunable synthesis of carbon nanotubes via methane catalytic pyrolysis by adjusting Mo incorporation in Fe/MgO

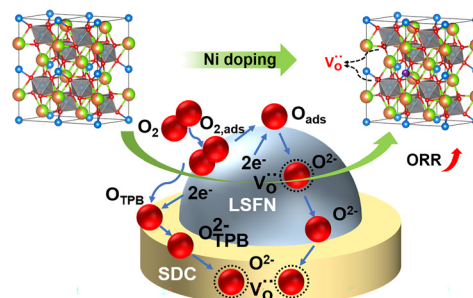
Zeyou Pan, Frank Krumeich, Paweł P. Ziemiański and Jeroen A. van Bokhoven*



18309

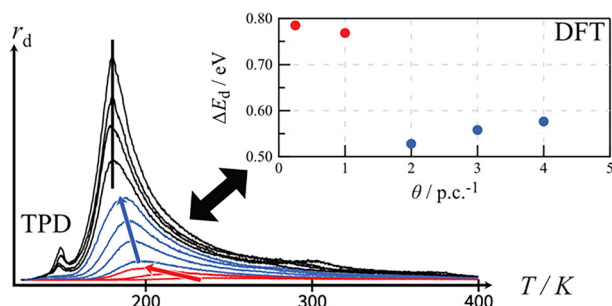
Regulation of electronic and ionic transport in Ni-doped $\text{La}_{0.6}\text{Sr}_{0.4}\text{FeO}_{3-\delta}$ for enhanced oxygen reduction in intermediate-temperature solid oxide fuel cells

Yuanyuan Ma, Songbo Li,* Zhen Yan, Shengli An, Hongli Qiao, Yanpeng Liu, Jing Zhang, Xu Zhang, Guangrui Zhang and Jing Zhao



RESEARCH PAPERS

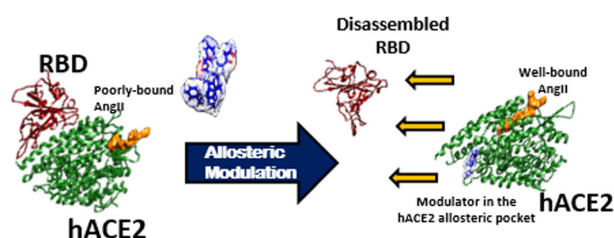
18317



Water desorption from microcline (001): insights into the first water layer

Tobias Dickbreder,* Florian Schneider, Lea Klausfering, Kim Noelle Dreier, Franziska Sabath, Adam S. Foster, Ralf Bechstein and Angelika Kühnle

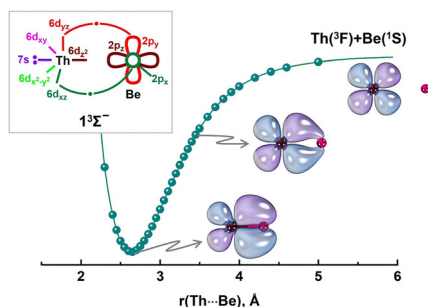
18326



Modulating functional allostery of the host-cell receptor protein hACE2 to inhibit viral entry of SARS-CoV-2

Pratyush Pani, Saroj Kumar Panda and Malay Kumar Rana*

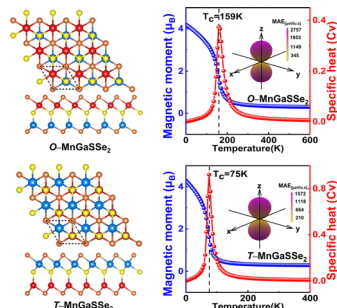
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Ground and excited state properties of ThBe and AcBe

Isuru R. Ariyaratna

18351



Possible transformation between half-metallic and metallic states of multiferroic MnGaSSe₂ monolayers

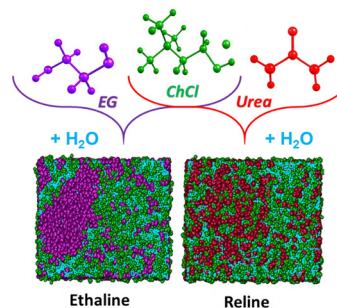
Zhiwen He, Shu Wang, Xue Rui, Jun Zhu, Yi Sun,* Jinlian Lu, Xueke Yu* and Xiuyun Zhang*



18358

Structural and interfacial behavior of choline chloride-based DESs (CholCl:EG and CholCl:urea) at various weight percentages in water mixture

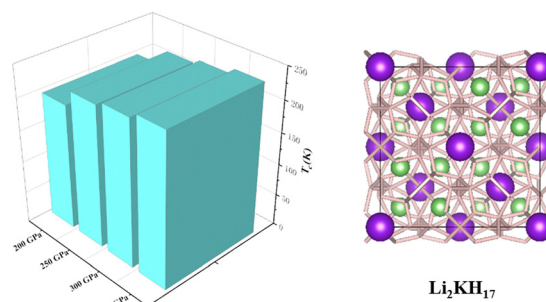
Rokhsareh Khodabandeh and Amin Reza Zolghadr*



18379

Superconducting properties of Li₂KH₁₇ with a cage configuration under high pressure

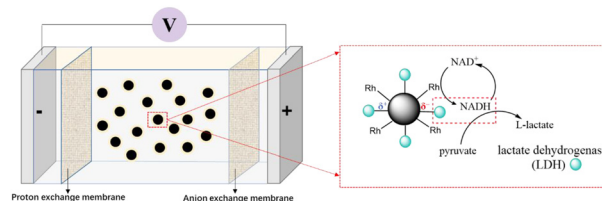
Qiyu Fu, Yuhang Wang, Xuejiao Xu, Wenhua Li, Xuyan Xue, Wei Zhang, Wencai Lu, Huijuan Sun* and Wenhua Yang*



18387

Co-immobilization of a rhodium catalyst and LDH on a carbon electrode using a covalent graft strategy for electrosynthesis of L-lactate in a bipolar electrochemical system

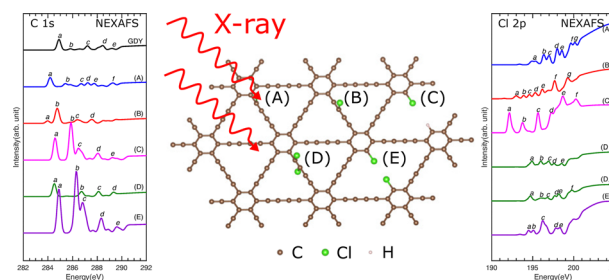
Chunhua Zhang,* Bowen Li,* Xiang Gao, Wei Xiao, Mingfang Chen and Qilong Bian*



18395

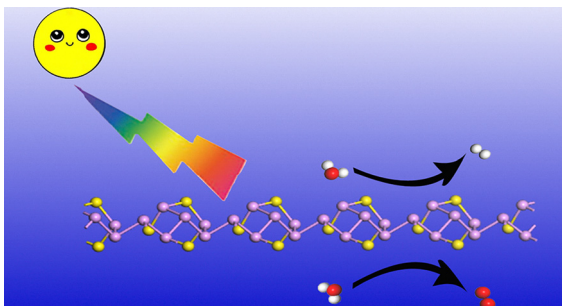
Unveiling the structure of chlorine-doped graphdiyne via first-principles X-ray spectroscopy

Hao-Qing Zhu, Hai-Bo Li, Xiu-Neng Song and Yong Ma*



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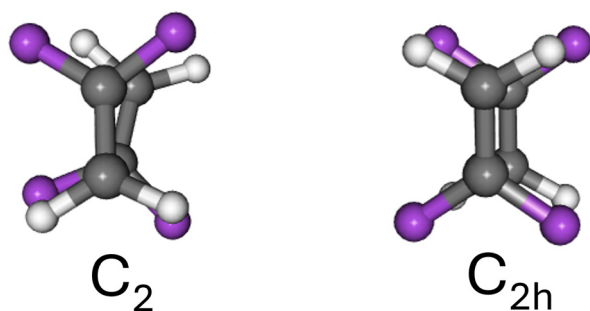
18403



Two-dimensional P₂S-I monolayer as a promising photocatalyst for overall water splitting

Xuan Li, Li Shao,* Yanli Yang, Yuantao He, Yan Li and Jiehu Cui*

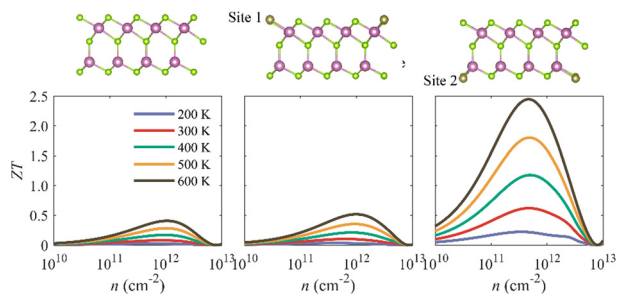
18409



Low temperature jet spectra of (DFE)₂, DFE-He, DFE-He₂ and DFE in the 2210–3105 cm⁻¹ region (DFE = 1,1 difluoroethylene)

A. J. Barclay, A. R. W. McKellar, A. Pietropolli Charmet and N. Moazzen-Ahmadi*

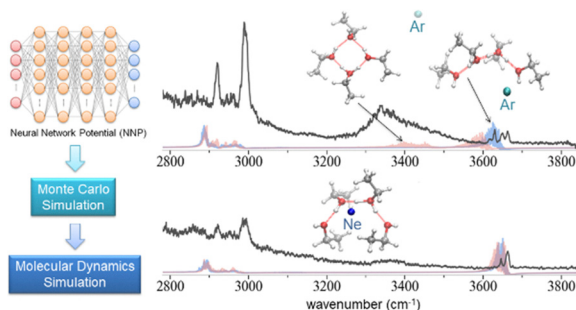
18420



Boosting thermoelectric performance of ferroelectric monolayer α -In₂Se₃ via strongly enhanced phonon scattering induced by site-specific Te doping

Weinan Zheng, Xinyang Li, Qiuyun Wang* and Anmin Chen*

18430



Linear–cyclic isomer competition in protonated ethanol–methanol clusters probed by infrared spectroscopy and deep-learning structural and dynamical simulations

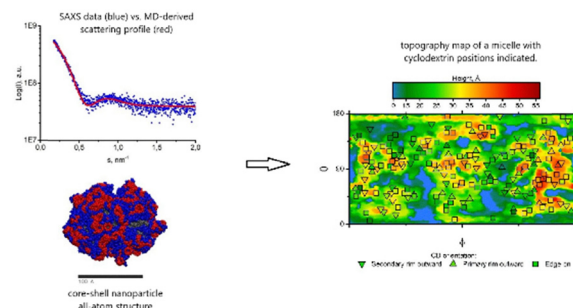
Po-Jen Hsu, Atsuya Mizuide, Jer-Lai Kuo* and Asuka Fujii*



18444

Arrangement and dynamics of individual cyclodextrins on the surface of core-shell micelles

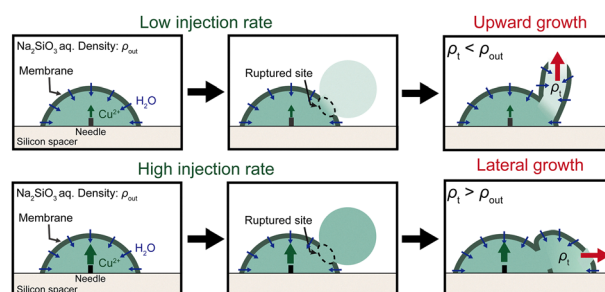
I. S. Vaskan,* V. A. Dimitreva, A. A. Piryazev, E. N. Subcheva, N. V. Bovin, A. B. Tuzikov, V. A. Oleinikov and A. V. Zalygin*



18454

Injection rate control on the growth direction in chemical gardens

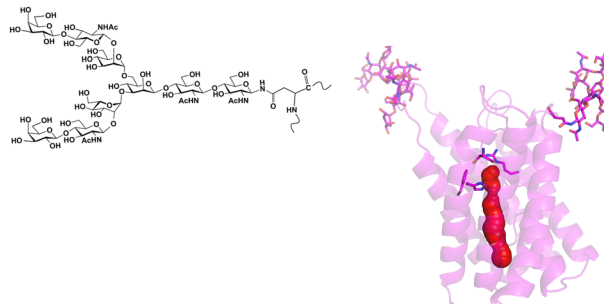
Yujin Kubodera, Muneyuki Matsuo and Satoshi Nakata*



18459

Mechanistic insights into glycosylation-driven structural rearrangements in human aquaporin 1

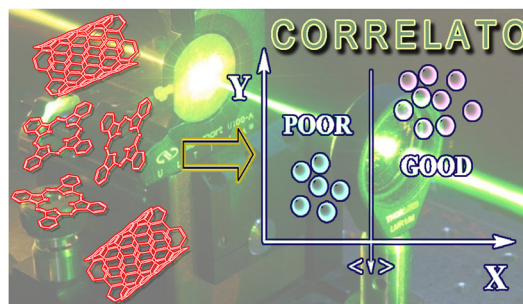
Keisuke Saito,* Yasuhiro Kajihara* and Hiroshi Ishikita*



18467

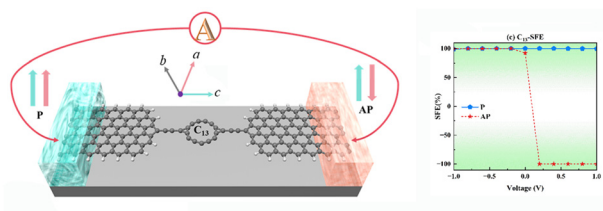
Intelligent methods for assessing the efficiency of optical limiters based on carbon nanomaterials using the CORRELATO approach

Alexander Yu. Tolbin,* Bogdan A. Tretyakov, Mikhail S. Savelyev, Pavel N. Vasilevsky and Alexander Yu. Gerasimenko



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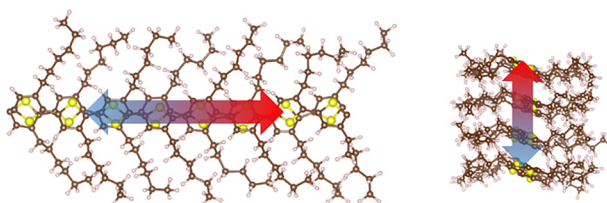
18478



Spin multifunctional transport properties of C_{13} and C_{14} molecule-based molecular nanodevices

Shenlang Yan,* Songbo Xiong, Tong Chen and Mengqiu Long

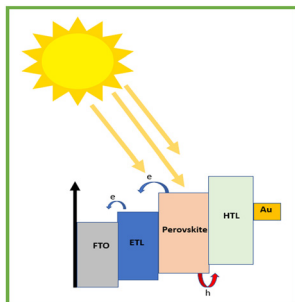
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Heat transfer through covalent *versus* non-covalent bonding: a case study on crystalline π -conjugated P3HT polymer using approach-to-equilibrium molecular dynamics

Cheick Oumar Diarra, Carlo Massobrio and Evelyne Martin*

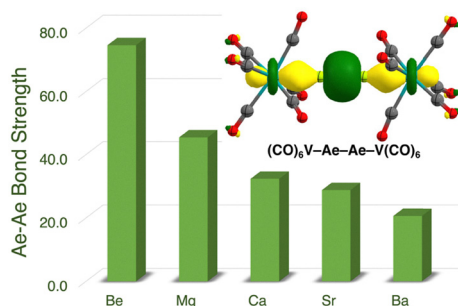
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Impact of Ce doping on the optoelectronic and structural properties of a $CsPbI_2Br_2$ perovskite solar cell

M. I. Khan,* Ali Mujtaba, Mahvish Fatima, Riadh Marzouki, Saddam Hussain and Tauseef Anwar

18504



Hepta-coordinated vanadium stabilized alkaline earth dimers: a DFT study

Ranjit Saha* and Pratim Kumar Chattaraj*

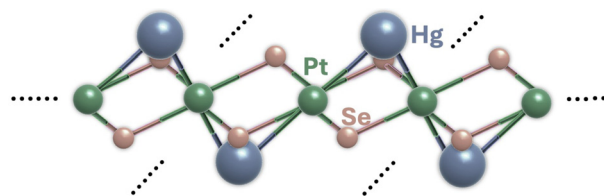


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18511

Quantized optical conductivity of gated and irradiated monolayer Pt_2HgSe_3

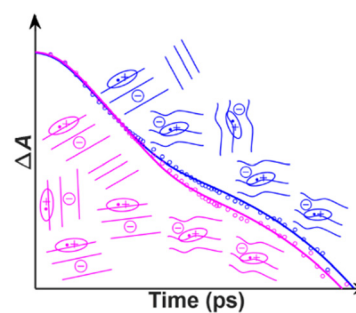
Bui D. Hoi* and Ta T. Tho



18517

Effect of local chain ordering on macroscopic charge mobility in chemically doped P3HT

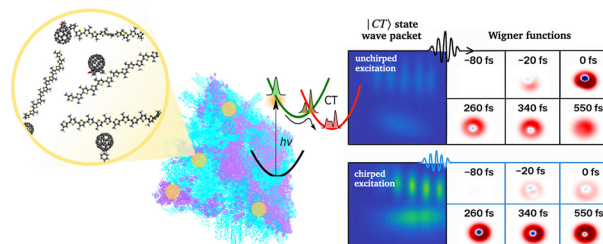
Abdul Rashid Umar, Adib Taba, Masoud Mahjouri-Samani and Christopher Grieco*



18525

Extending quantum coherence lifetimes in nonadiabatic dissipative molecular systems with chirped pulses

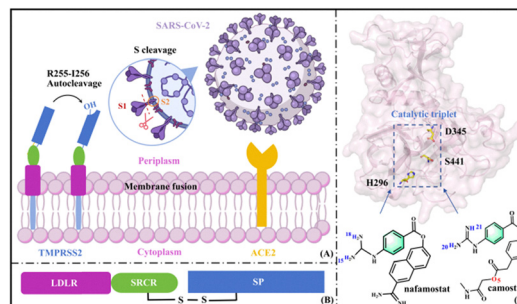
Robert Strich, Shirin Faraji and Elisa Palacino-González*



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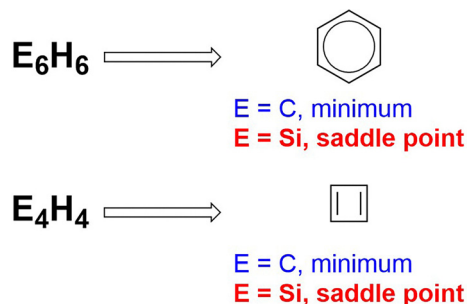
Difference in the inhibitory mechanism against TMPRSS2 between camostat and nafamostat: implications for drug design

Tiantian Yang, Wentong Yu, Du Guo, Jing Li, Xinmin Wang, Yuting Song, Yan Cheng, Yuxi Luo, Jianghua Yang, Weiwei Ouyang* and Jianping Hu*



RESEARCH PAPERS

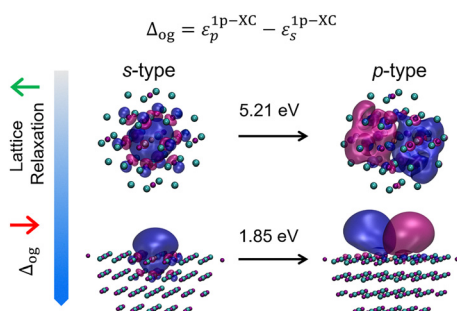
18555



Aromaticity and antiaromaticity in the cyclic 6π and 4π molecules of carbon and silicon E_6H_6 and E_4H_4 (E = C, Si)

Lili Zhao, Qin Ma, Israel Fernández* and Gernot Frenking*

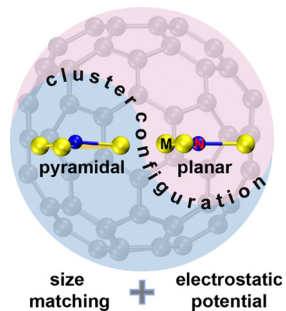
18567



Optical gaps of F-center defects in LiF using many-body methods

Ritaj Tyagi, Abhisek Ghosal and Vamsee K. Voora*

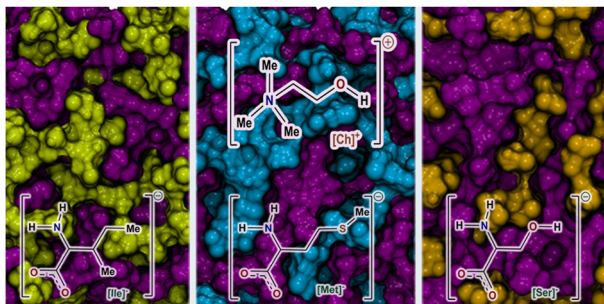
18577



Size matching and electrostatic potential as complementary methods for understanding the metallic cluster configurations inside fullerenes

Chenliang Pan, Shuaijiang Liu and Peng Jin*

18586



Tailoring ionic liquid properties via amino acid anions: structural influence of isoleucine, methionine, and serine anions

Sonia Yadav and Anurag Prakash Sunda*

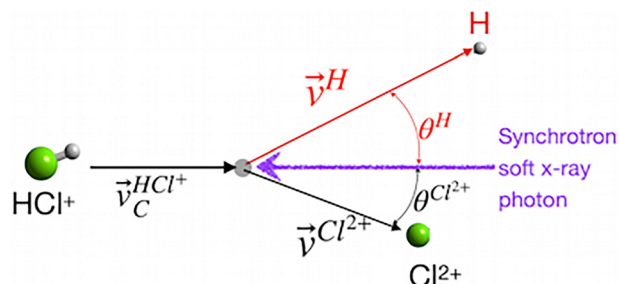


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18595

Ionic photofragmentation cross sections of the HS^+ , H_2S^+ and HCl^+ molecular ions near the 2p threshold

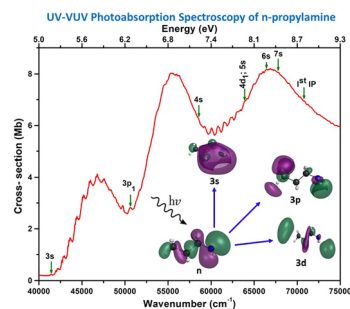
Jean-Paul Mosnier,* Eugene T. Kennedy,
Denis Cubaynes, Jean-Marc Bizau,
Ségolène Guilbaud and Stéphane Carniato



18609

UV-VUV absorption spectroscopy and photodissociation dynamics of *n*-propylamine

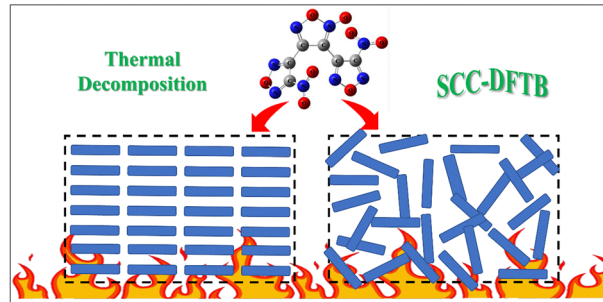
Neha Sharma, Aparna Shastri,* Asim Kumar Das,
Vandana Rawat and Balabhadrapatruni Naga Rajasekhar



18626

Molecular packing-dependent thermal decomposition pathways in 3,4-dinitrofurazanfuroxan: insights from SCC-DFTB molecular dynamics simulations

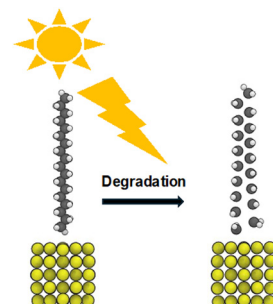
Shuangfei Zhu,* Fangfang Hou, Jinxuan Xue,
Ruijun Gou, Shuhai Zhang,* Shangbiao Feng and
Yang Liu



18635

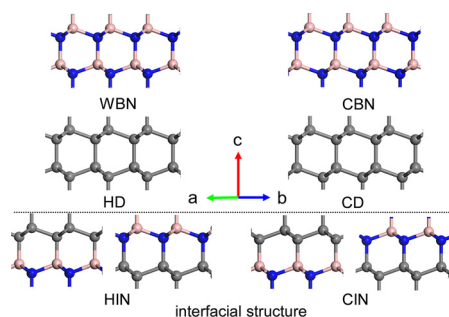
Plasmonic degradation of plastics on gold nanoparticles: electronic-scale insights from computation

Hajar Hosseini, Connor J. Herring, Noshir S. Pesika and
Matthew M. Montemore*



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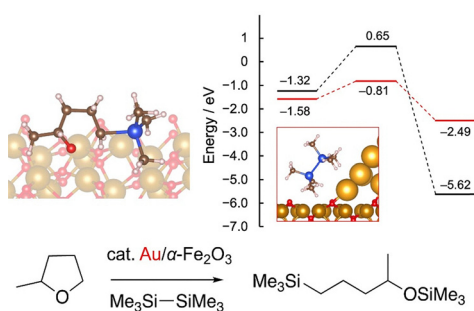
18645



Examining the stability and mechanical characteristics of interface structures within diamond/BN composite materials

Qi Gao,* Li Zhu, Kun Luo,* Lingjuan Hao, Feifei Ling, Chao Ren, Xianda Han, Xiaogang Guo, Zhixuan Chen, Julong He and Dongli Yu

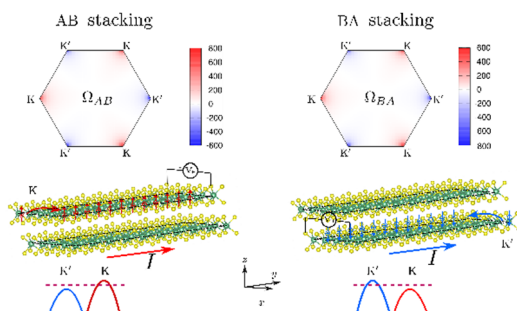
18651



Reaction mechanism of silylation of C–O bonds in alkyl ethers over supported gold catalysts: experimental and theoretical investigations

Yunosuke Tsunesada, Tatsushi Ikeda, Koki Muraoka, Masafumi Doi, Hiroki Miura,* Tetsuya Shishido* and Akira Nakayama*

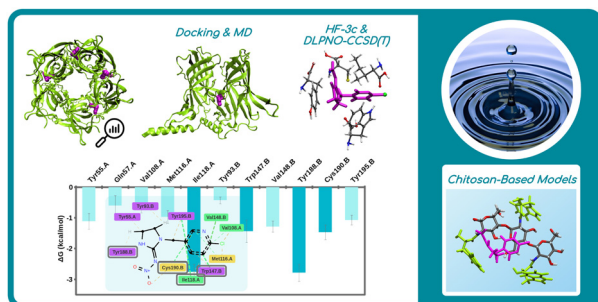
18658



Electrically switchable valley polarization and an anomalous valley Hall effect in monolayer and bilayer NbS₂

Zhifan Zheng, Tengfei Cao, Chun-Sheng Liu, Xiaohong Zheng,* Hua Hao,* Yushen Liu* and Shaohui Yu

18665



Towards nature-inspired materials for adsorbing pesticides: a multi-stage computational approach

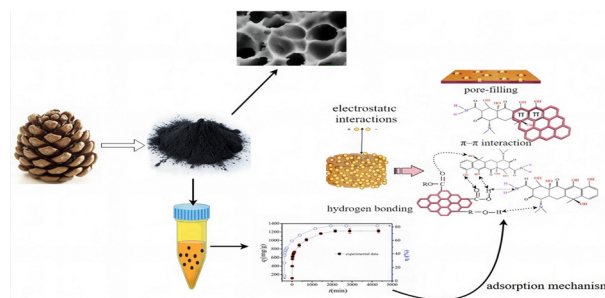
J. R. C. Santos, P. E. Abreu and J. M. C. Marques*



18681

Three-dimensional hierarchical porous P,O co-doped pinecone biochar for tetracycline removal: behavior and mechanism

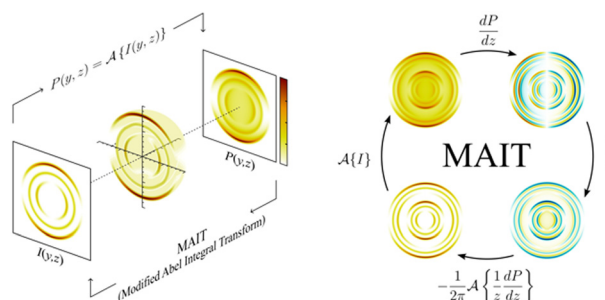
Jianfang Lu, Chaojie Fan, Yuanyuan Huang, Pengfei Li, Fuhou Lei, Haitang Xu, Caiyun Han, Kechun Li* and Yu Feng*



18694

Revisiting the inverse Abel integral for reconstructing velocity-map images

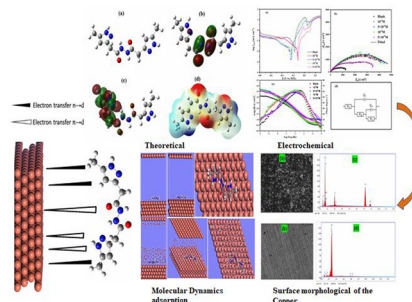
Chris Sparling* and Jolijn Onvlee*



18710

Electrochemical and theoretical insights into Schiff base derivatives for the prevention of copper corrosion

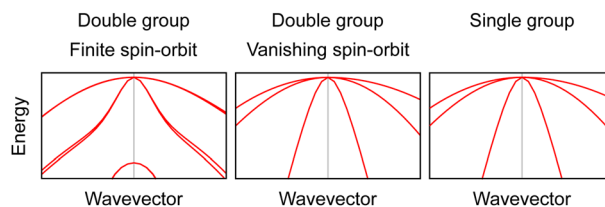
Mohammed Lasri,* Abouelhaoul El Alami, Nouredine Idlahoussaine, Aziz Ait-Karra, Othmane Zakir, Mohamed Maatallah, Rachid Idouhli, Rabiaa Fdil, Mohy Eddine Khadiri and Abdesselam Abouelfida



18723

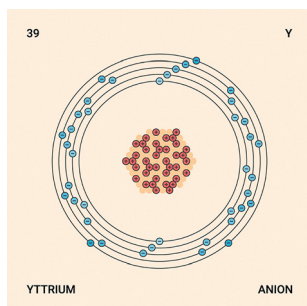
Kramers degeneracy originates from two time-reversal symmetries

Koshi Okamura



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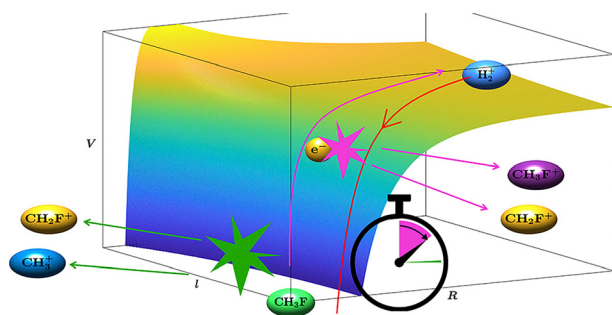
18734



Understanding the binding in excited states of the yttrium anion

Maria Barysz

18741

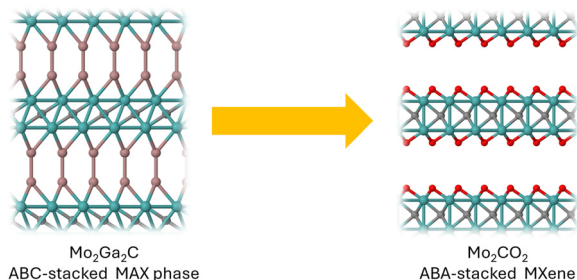


Competition between electron transfer and reactive capture in ion–molecule reactions at low collision energies: isotopic and stereodynamic effects in the reactions of CH_3F with H_2^+ , HD^+ and D_2^+

Raphaël Hahn, David Schlander, Jeremy O. Richardson, Timothy P. Softley and Frédéric Merkt*

18760

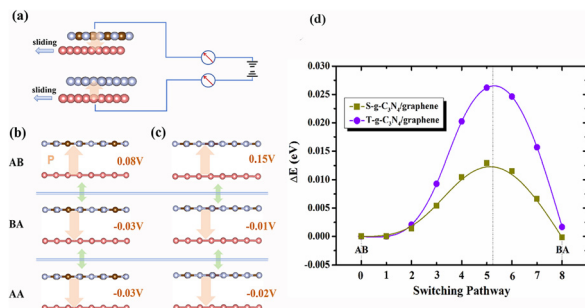
Oxygen-aided Ga etching and ABC-to-ABA phase transition



The role of oxygen in the synthesis of the Mo_2CT_x MXene from the $\text{Mo}_2\text{Ga}_2\text{C}$ MAX phase

José D. Gouveia* and José R. B. Gomes*

18770



Sliding ferroelectricity and alterpiezoelectricity in a two-dimensional heterobilayer from the in-plane hole of $g\text{-C}_3\text{N}_4$

Yuhua Wei, Feng Gao,* XuLi Cheng, HaoTian Wang, YingJie Hu, ZuHui Hu, Hui Zhang, Jin Wen, Yin Wang* and Wei Ren*

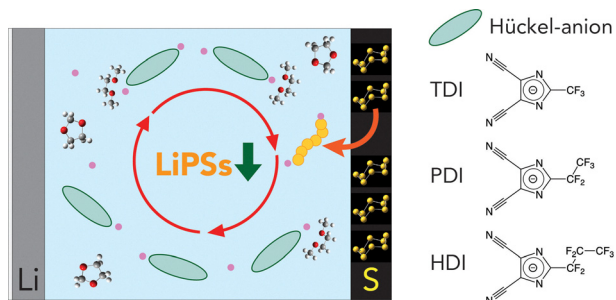


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18778

Hückel anion based concentrated electrolytes for lithium–sulfur batteries

Aginmariya Kottarathil,* N. Tan Luong, Carolina Cruz Cardona, Steffen Jeschke, Tomooki Hosaka, Grażyna Zofia Żukowska, Maciej Marczewski, Władysław Wiczorek and Patrik Johansson*

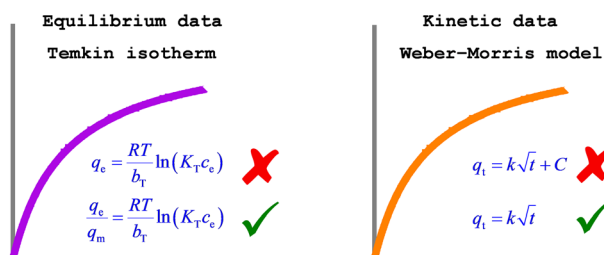


COMMENTS

18789

Comment on “Unravelling the kinetics, isotherms, thermodynamics, and mass transfer behaviours of Zeolite Socony Mobil – 5 in removing hydrogen sulphide resulting from a dark fermentative biohydrogen production process” by M. K. A. Asman *et al.*, *Phys. Chem. Chem. Phys.*, 2024, 26, 20409

Khim Hoong Chu,* Mohd Ali Hashim and Mohd Hafiz Zawawi

H₂S adsorption on zeolite

18793

Reply to the ‘Comment on “Unravelling the kinetics, isotherms, thermodynamics, and mass transfer behaviours of Zeolite Socony Mobil – 5 in removing hydrogen sulphide resulting from a dark fermentative biohydrogen production process”’ by K. H. Chu, M. A. Hashim and M. Hafiz Zawawi, *Phys. Chem. Chem. Phys.*, 2025, 27, DOI: 10.1039/D4CP04682J

Muhammad Khairul Adha Asman, Nabilah Aminah Lutpi,* Yee-Shian Wong, Soon-An Ong, Muhammad Adli Hanif, Naimah Ibrahim, Farrah Aini Dahalan, Wirach Taweepreda and Raja Nazrul Hakim Raja Nazri

