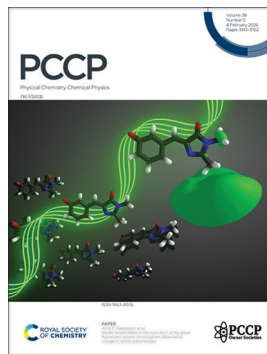


IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 28(5) 3143–3762 (2026)



Cover
See Osamu Shirai *et al.*, pp. 3161–3167.
Image reproduced by permission of Osamu Shirai from *Phys. Chem. Chem. Phys.*, 2026, 28, 3161.



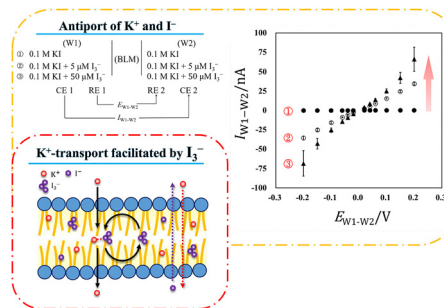
Inside cover
See Anne P. Rasmussen *et al.*, pp. 3168–3173.
Image reproduced by permission of Anne P. Rasmussen from *Phys. Chem. Chem. Phys.*, 2026, 28, 3168.

RESEARCH PAPERS

3161

Ion transport across bilayer lipid membranes between two aqueous phases in the presence of iodide and triiodide ions

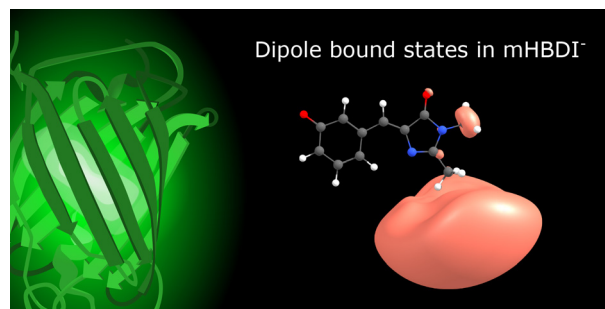
Weipai Chuang, Keisei Sowa, Yuki Kitazumi and Osamu Shirai*



3168

Dipole-bound states in the *meta* form of the green fluorescent protein chromophore observed by cryogenic action spectroscopy

Anne P. Rasmussen,* Nikolaj Klinkby and Lars H. Andersen



**GOLD
OPEN
ACCESS**

EES Solar

**Exceptional research on solar
energy and photovoltaics**



Part of the EES family

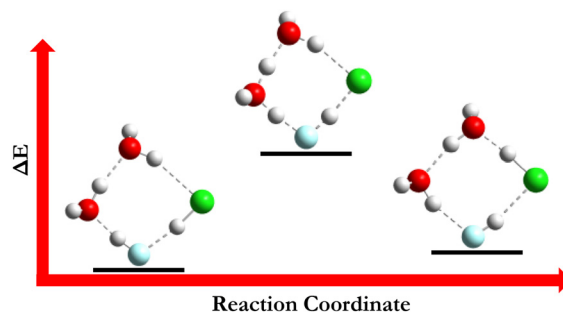
**Join
in** | Publish with us
rsc.li/EESolar

RESEARCH PAPERS

3174

Concerted proton transfer in homogeneous and heterogeneous cyclic hydrogen-bonded clusters of H₂O, HF, and HCl

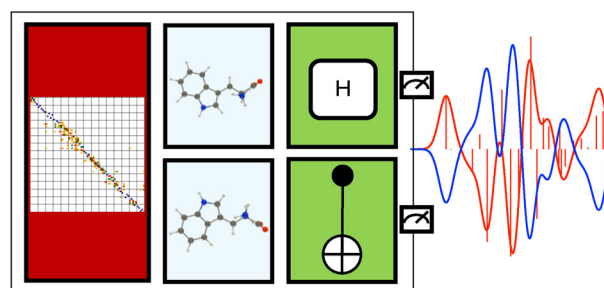
Max R. Tucker, Yuan Xue, Nathan R. Speake, Eden Nickolson, Jeremy M. Carr and Gregory S. Tschumper*



3183

A hybrid classical-quantum algorithm to simulate ECD spectra – the case of tryptophan zwitterions in water

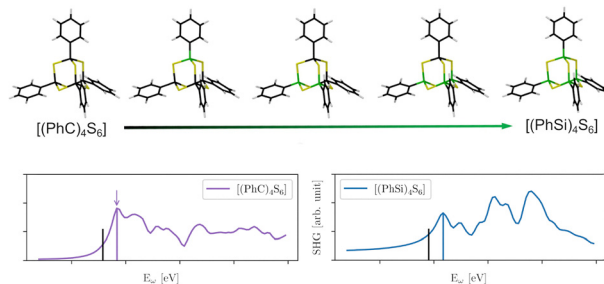
Renato Olarte Hernandez, Armand Soldera and Benoît Champagne*



3193

C atoms versus Si atoms at the bridgehead positions of phenyl-decorated adamantane-type clusters: influence on the nonlinear optical response

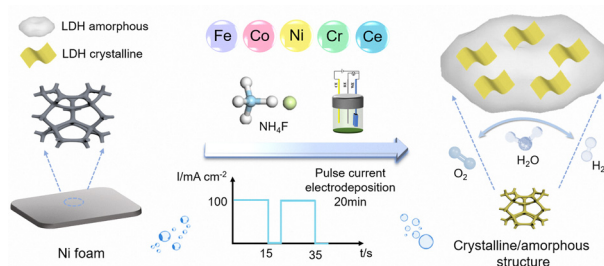
Ferdinand Ziese, Stefanie Dehnen and Simone Sanna



3204

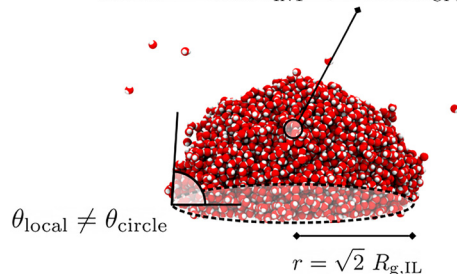
High-entropy FeCoNiCrCe layered double hydroxides by facile pulse current electrodeposition as high performance electrocatalysts for the oxygen evolution reaction

Xinyu Yang and Qianqiao Chen*



3213

$$\text{RMSD}^2 = \text{RMSD}_{\text{INT}}^2 + 2 \text{RMSD}_{\text{CPL}} + \text{RMSD}_{\text{COM}}^2$$

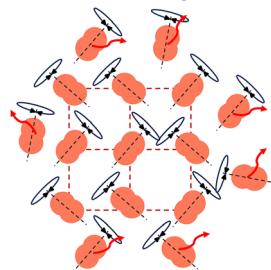


Robust methods for the characterization of droplet behavior in molecular dynamics: from contact radius to contact angle

Farshad Esmailian,* Morteza Torabi Rad, Masumeh Foroutan* and Mikko Karttunen*

3227

Heterogeneous translational dynamics
in core and surface regions



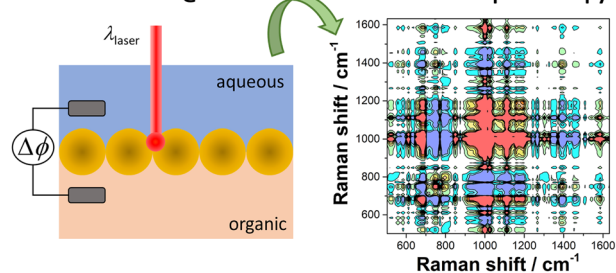
Heterogeneous translational dynamics of succinonitrile in the plastic crystalline phase

Keiko Nishikawa* and Kozo Fujii

3236

EC-SERS@ITIES

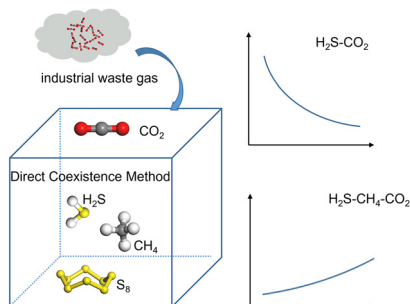
2D Correlation Spectroscopy



2D correlation SERS of organic ions using AuNP films at electrified soft interfaces

Madjid Tarabet, Yinxi Zou, Dyia Syaleyana Md Shukri, Noorfatimah Yahaya, Manuel Dossot* and Grégoire Herzog*

3245



Dual regulatory roles of CO₂ on molecular sulfur dissolution in sour components of high-sulfur natural gas: insight from molecular dynamics simulations

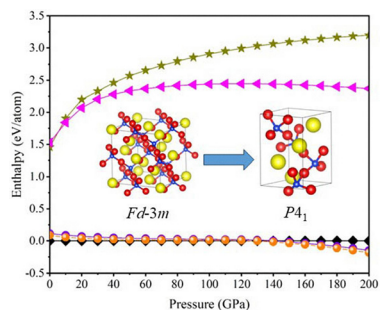
Shuangli Yue, Nong Li, Li Wang,* Ying Wan, Chengxin He, Li Zhang* and Mingli Yang



3255

Prediction of radon-silica systems in the Earth's mantle

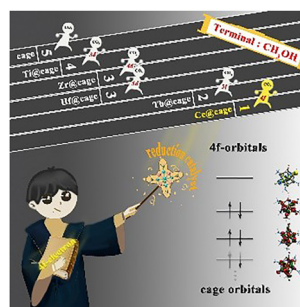
Kai Hu, Yixing Geng, Yanying Zhao, Yuqiu Gu,*
Jinqing Yu* and Xueqing Yan*



3262

4f-Electron localization in Ce-embedded Co_6Te_8 clusters for enhanced CO_2 reduction catalysis

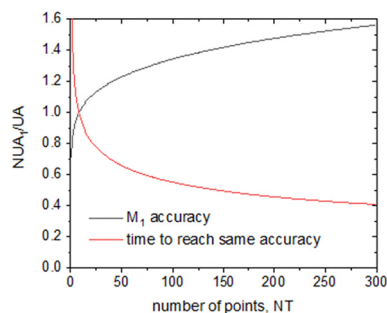
Zhiyuan Zhang, Jiarui Li, Pawel M. Kozlowski,
Wang Cong, Kamran Akbar, Yanning Zhang,*
Georg Schreckenbach,* Yang Gao* and Zhiming Wang



3272

Analytically optimized noise redistribution in pulsed dipolar EPR spectroscopy

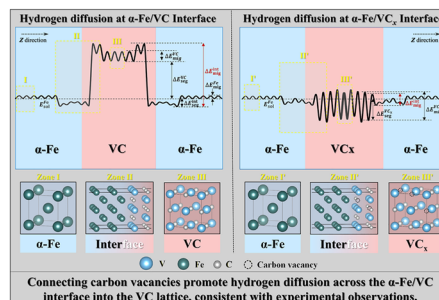
V. M. Nekrasov, A. G. Matveeva,* V. N. Syryamina,
S. A. Agarkin and M. K. Bowman



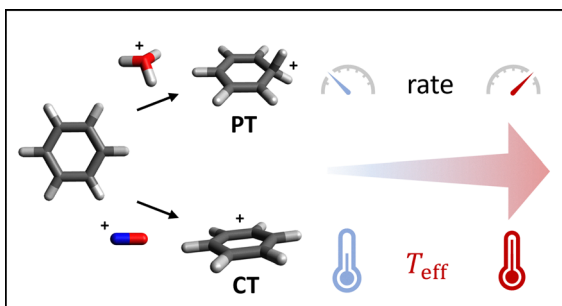
3282

Carbon vacancy network mediated hydrogen trapping at the α -Fe/VC interface

Linxian Li, Huifang Lan, Shuai Tang,* Fengliang Tan,
Qing Peng,* Zhenyu Liu and Guodong Wang



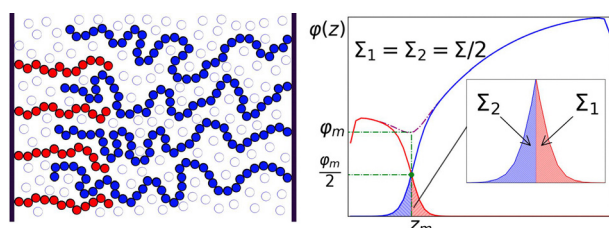
3291



Investigations on the field dependency of proton and charge transfer kinetics in atmospheric pressure corona discharge sources

Christoph Schaefer,* Alexander Haack,*
Charlotte Hellwig, Jannik Wuttke and
Stefan Zimmermann

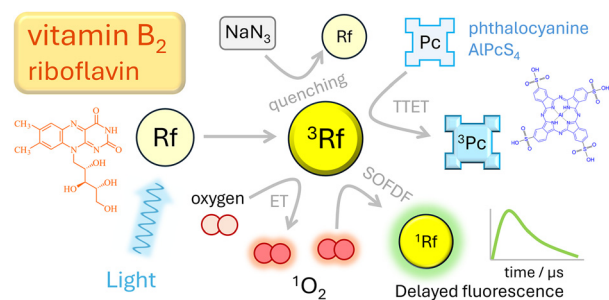
3305



Compressed asymmetric polymer brushes exhibit a symmetric interpenetration zone

Leonid I. Klushin, Ivan V. Lukiev, Ivan V. Mikhailov,*
Oleg V. Borisov and Aleksander M. Skvortsov

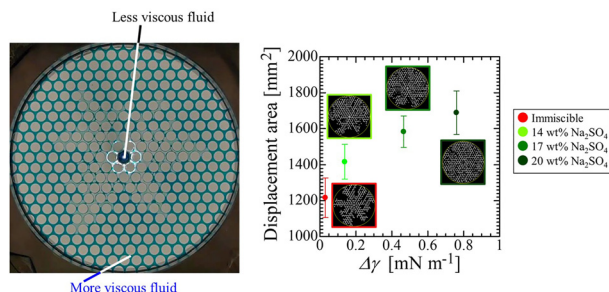
3316



Riboflavin – understanding the dynamics and interactions of the triplet state

Marek Scholz, Jan Moučka, Jakub Pšenčík, Jan Hála and
Roman Dedic*

3325



Experimental demonstration of enhanced displacement by phase separation in a two-dimensional milli-model in viscously unstable fluid displacement

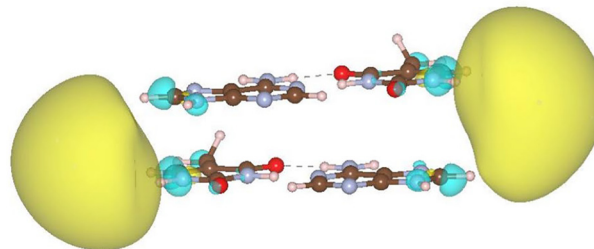
Shunta Kiuchi, Yuichiro Nagatsu, Takahiko Ban,
Manoranjan Mishra and Ryuta X. Suzuki*



3336

Nature of frontier quasi-particle states in nitrogen-base systems

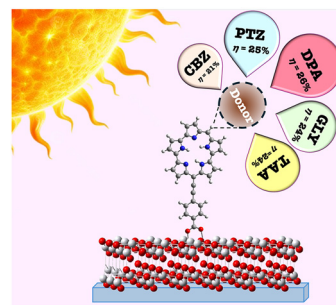
Raul Quintero-Monsebaiz, Per Hyldgaard and Elsebeth Schröder*



3352

Molecular engineering of antiaromatic orangarin-based sensitizers for high-performance dye-sensitized solar-cell applications

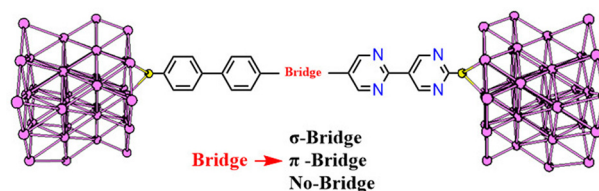
Swati Singh Rajput, Samarth Razdan, Tejendra Banana, Neelam Chandravanshi and Md Mehboob Alam*



3363

Effect of bridge type on electronic structure and rectification in molecular junctions

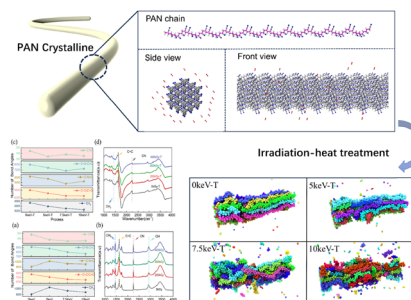
Morad M. El-Hendawy,* Hend S. Abd Elkhair and Mahmoud M. A. Mohamed



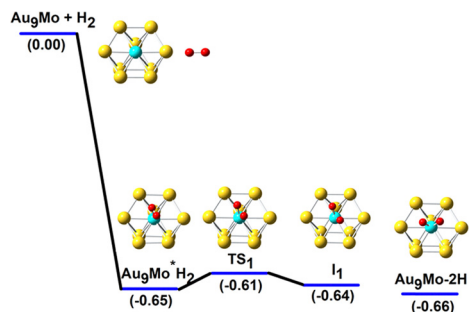
3375

Defect evolution and molecular transformation in the crystalline region of polyacrylonitrile fibers during irradiation-heat pre-oxidation: integrated simulation and experimental study

Meng Wu, Ruiqi Shao,* Amna Siddique,* Nishonov Akbarjon,* Tianyu Li, Tianshuai Ma, Shouguo Liu, Wei Wang and Zhiwei Xu*



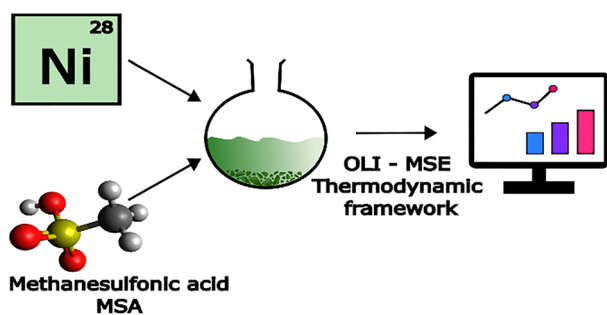
3389



DFT investigation of Au_nMo ($n = 2-12$) clusters: the barrierless hydrogen adsorption behavior of Au_9Mo

Ngo Thi Lan, Nguyen Van Dang,* Nguyen Thi Mai, Son Tung Ngo and Nguyen Thanh Tung

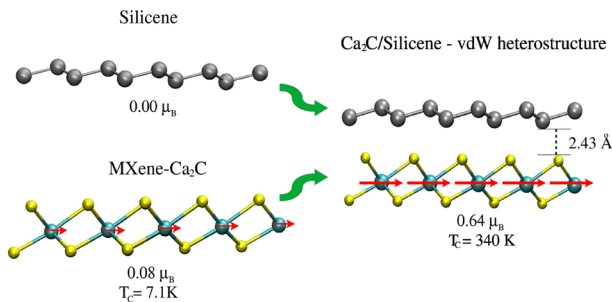
3401



Phase equilibria and thermodynamic properties of the nickel(II) methanesulfonate–methanesulfonic acid–water system

Femke Derison, Xu Jia, Luc Van Meervelt, Koen Binnemans and Rayco Lommelen*

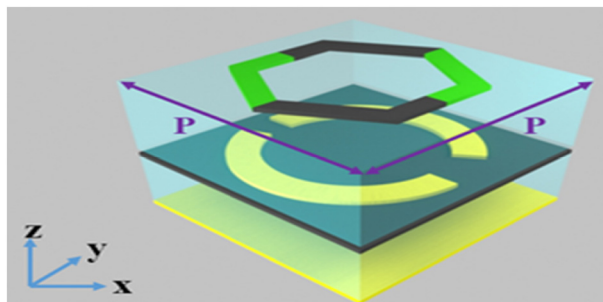
3415



Enhancing the magnetic properties (Curie temperature and magnetic anisotropy energy) of a 2D MXene (Ca_2C) by stacking a vdW heterostructure with silicene

Jonas Anversa, Rogério José Baierle* and Paulo César Piquini

3423



A dynamically reconfigurable terahertz metasurface enabled by hybrid $Ge_2Sb_2Te_5$ and VO_2 phase-change materials

Guan Wang,* Mingna Chu, Jijuan Jiang, Yang Jia, Jia Liu, Hailong Yu, Hongyan Meng and Wenqiang Shi

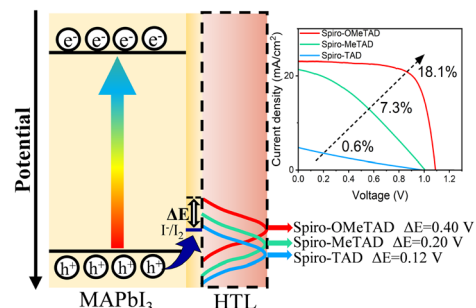


RESEARCH PAPERS

3434

Regulating the electrode potential offset in perovskite solar cells for boosting interfacial charge transfer

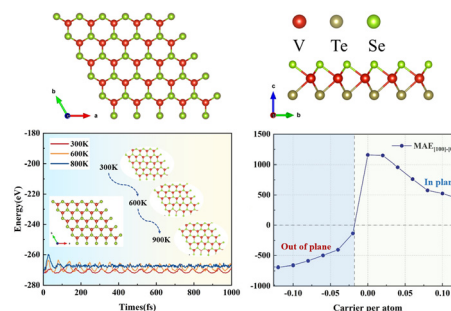
Qiong Wang, Mengfan Xue, Kaijian Zhu, Qiyu Qu, Bo Wang, Shengyao Wang,* Bing Wang, Zhigang Zou and Wenjun Luo*



3442

Electronic structure and magnetothermal properties of the Janus VSeTe monolayer manipulated by carrier doping

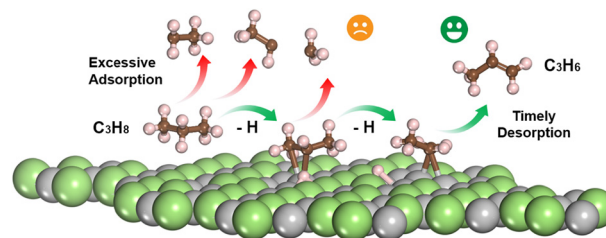
Yue Yang, Shuai-Kang Zhang, Jun-Kang Jiang, Cui-E Hu,* Hua-Yun Geng and Xiang-Rong Chen



3454

Ga-induced electronic tuning of Ni catalyst surfaces: achieving activity–selectivity balance in propane dehydrogenation

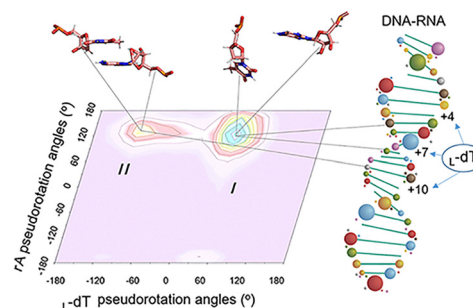
Zebing Bao, Xiaojing Duan, Xiaofeng Guo, Shouqi Zhang, Huibo Qin,* Linhai Duan,* Xiuhong Meng, Hanlu Wang and Xingyuan Chen



3467

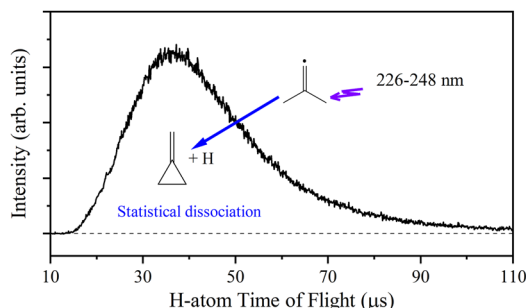
Theoretical investigation into the position-dependent influence of L-deoxynucleotides in the template strand on T7 RNA polymerase transcription activity

Xuyang Ma, Yongqi Ke, Xinping Feng, Yang Zhang, Qingju Liu, Yujian He, Wei Cui* and Li Wu*



RESEARCH PAPERS

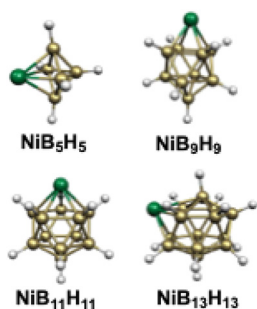
3481



H atom product channels in the ultraviolet photodissociation of the 2-methyl-1-propenyl radical

Michael Lucas, Yuan Qin, Lei Yang, Ge Sun and Jingsong Zhang*

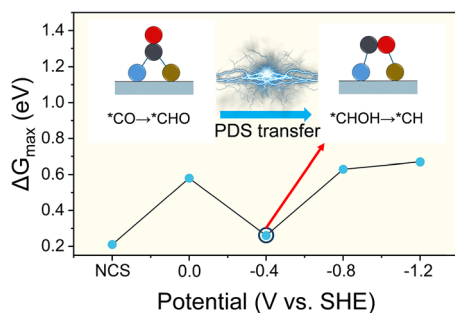
3490



Bare group 10 metal atoms as vertices in polyhedral metallaboranes: spherical aromaticity in the icosahedral MB₁₁H₁₁ systems

Amr A. A. Attia, Alexandru Lupan* and R. Bruce King*

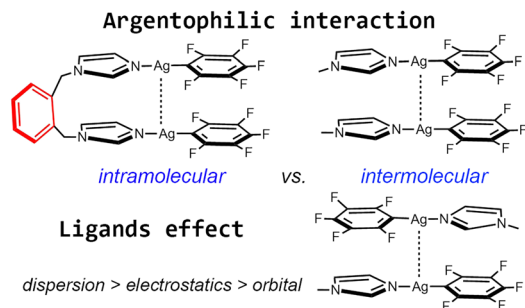
3501



Electrochemical potential-driven evolution of *CO electronic structure and adsorption configuration on Te-based diatomic catalysts for enhanced CO₂ reduction

Yiming Yang, Xiaolong Li, Chengwei Yang, Guixian Ge* and Yanwen Zhang*

3511



Unveiling the nature of ligand-modulated argentophilic interactions: a theoretical study of intra- and intermolecular silver complexes

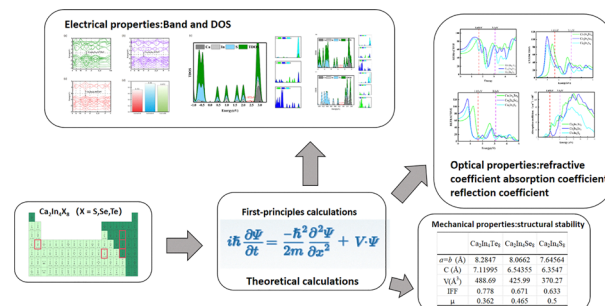
Yuan Xu,* Shan Liao and Peifeng Su



3521

A theoretical study of the photoelectric properties of lead-free $\text{Ca}_2\text{In}_4\text{X}_8$ ($\text{X} = \text{S}, \text{Se}, \text{Te}$) via density functional theory

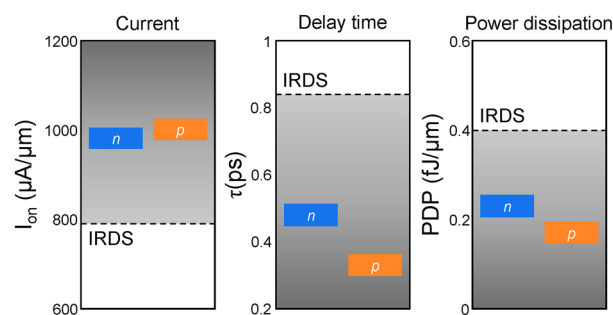
Wenbin Zhu, Beitong Cheng, Changcheng Chen,* Yue Cheng, Shuaikang Zhang, Kunzhuo Zhao, Zhengjun Wang, Xinhui Zhang, Chunling Zhang, Jiangzhou Xie, Yaxin Xu, Xiaoning Guan, Gang Liu* and Pengfei Lu*



3531

Monolayer Sc_2NF_2 and Sc_2NO_2 electrodes for bilayer MoS_2 : achieving symmetric and excellent performances

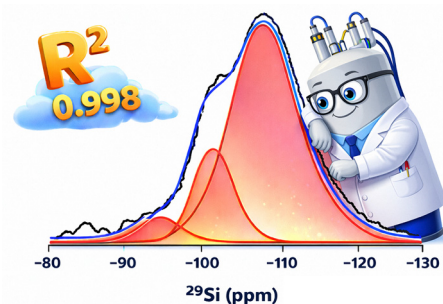
Hong Li,* Xiaotian Hu, Pengyang Liu, Fengbin Liu and Jing Lu*



3540

Quantitative ^{29}Si NMR spectroscopy of ordered mesoporous silicas: revisiting Q_3/Q_4 ratios and surface hydroxylation in SBA-15 and MCM-41

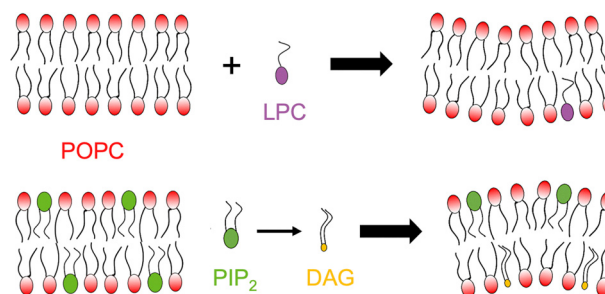
Valentina V. Sobornova and Ilya A. Khodov*



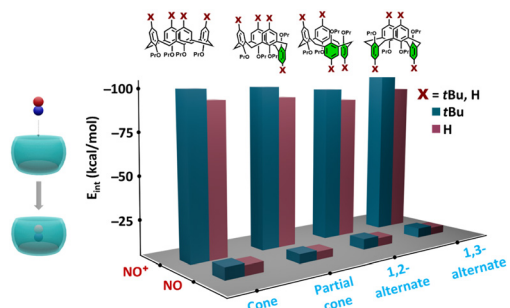
3550

Lipid bilayer membranes with asymmetrically distributed LPC and DAG

Chang Liu, Zhongjie Han, Rui Ma* and Chen Song*



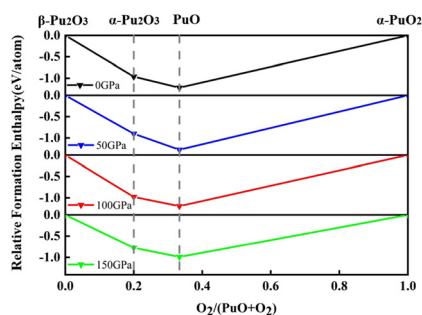
3562



Host-guest interaction of NO and NO⁺ species with calixerenes: dissecting the impact of conformational and confinement effects

Hadiya Mecheri Abdulla, Pookkottu K. Sajith,*
Subodh S. Khire and Karunakaran Remya

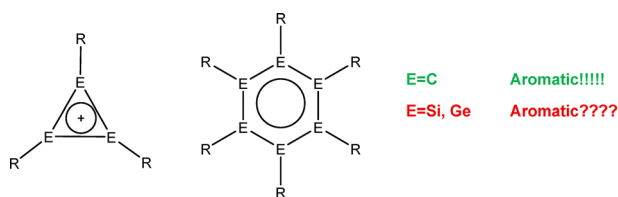
3576



High-pressure tuning of electronic structures, stability and mechanical properties of plutonium oxides: a DFT+U study

Xiaolin Zhang, Minzhuo Xiong, Jinxing Cheng,*
Qingbo Wang, Youpeng Wu and Ziyu Hu*

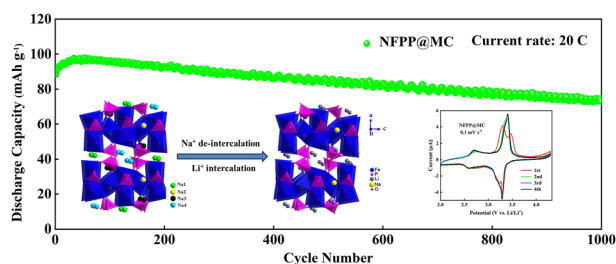
3588



The limit of the current aromaticity concept

Amnon Stanger,* Jordi Poater and Yirong Mo

3601



A low-cost and high-rate Na₄Fe₃(PO₄)₂P₂O₇@C cathode material directly used in lithium-ion batteries

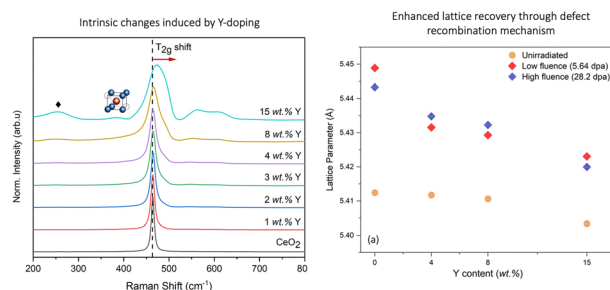
Zonghui Yi,* Hui Zhang, Zhiyuan Cheng, Lin Xie and Jiangping Cao



3613

Defect chemistry manipulation by heavy ion irradiation in Y-doped CeO₂ solid solutions

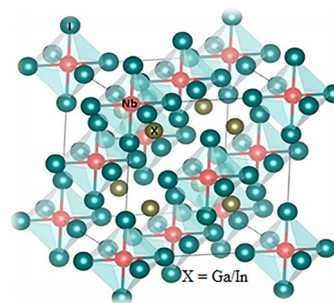
R. Mohun,* T. Cordara, J. McCloy, M. H. Weber, S. C. Middleburgh and C. L. Corkhill



3624

DFT analysis of the structural, electronic, magnetic and thermoelectric properties of X₂NbI₆ (X = Ga, In) vacancy-ordered double perovskites

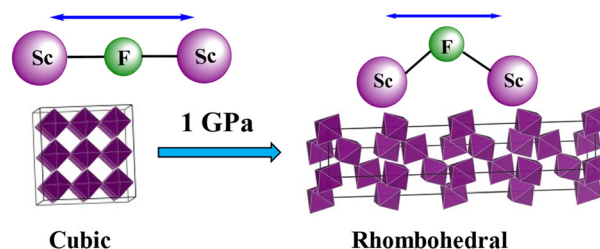
Afsar Ul Mulk, Malak Azmat Ali,* Jawad Hussain, Omar Alsalmi and Habib Ullah



3633

Anisotropic negative thermal expansion in high-pressure phases of ScF₃

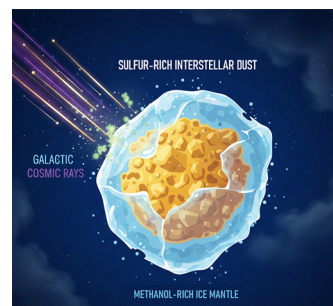
Soumya Mondal, Shovan Das and Ayan Datta*



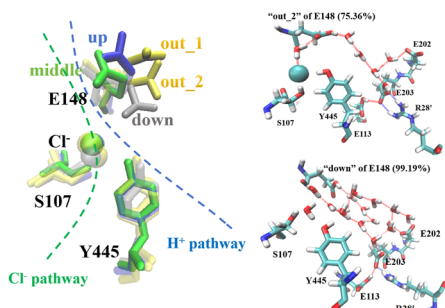
3642

Irradiation of methanol ice on a sulfur-rich dust analogue at 25 K: a mid-infrared spectroscopic study

D. V. Mifsud,* Z. Kaňuchová, O. Auriacombe, P. Herczku, R. Rácz, S. T. S. Kovács, D. Qasim, B. Sulik, Z. Juhász, I. Vajda, I. Rajta, U. Raut, S. Biri, S. Ioppolo and N. J. Mason*



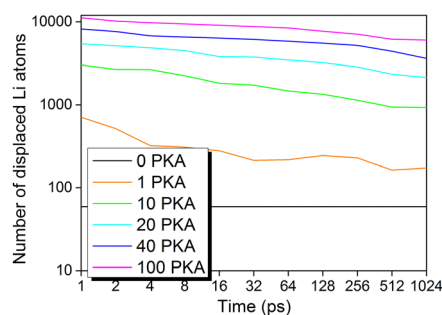
3656



Molecular dynamics investigation of the interaction between central-site chloride binding and proton transport in EcCLC

Zhe Wang,* Jiayi Zeng, Tao Yu and Lifeng Gao

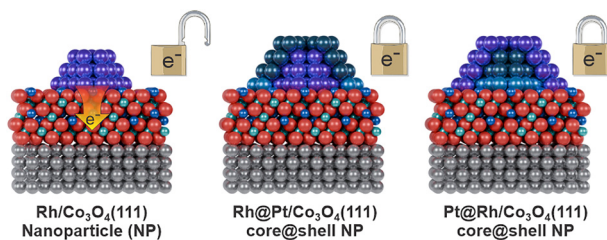
3668



Disorder and damage recovery in irradiated lithium oxide

M. Yu. Lavrentiev,* N. L. Allan and O. A. Hawkins

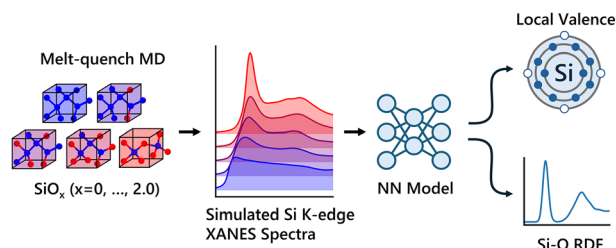
3675



A bimetallic strategy to modulate electronic metal support interaction in Co₃O₄(111)-based catalysts: the case of supported Rh–Pt core–shell nanoparticles

Jonas Hauner, Alexander Simanenkov, Lukáš Fusek, Tomáš Skála, Nataliya Tsud, Firas Faisal, Sascha Mehl, Jörg Libuda and Yaroslava Lykhach*

3682



Machine learning-based XANES analysis for predicting the local structure and valence in amorphous silicon suboxides

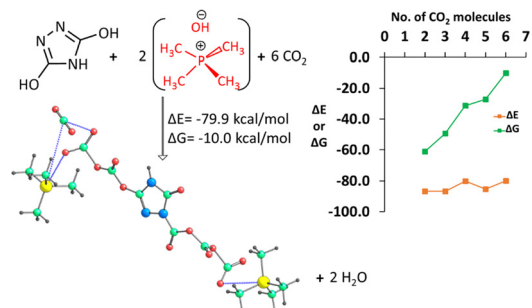
Yu Fujikata,* Hiroki Sugisawa and Teruyasu Mizoguchi



3693

Multi-site CO₂ fixation in triazolates: cooperative O,N binding enhanced by solvation and counter-ion effects

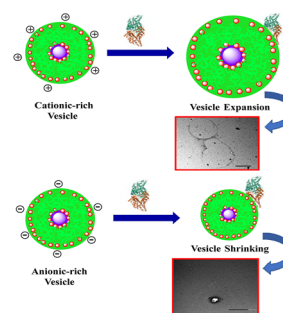
Puthiyavalappil K. Arathi, D. Sudha and Cherumuttathu H. Suresh*



3702

Electrostatic control of protein-vesicle interactions in cationic long-chain ionic liquid systems: insights from human serum albumin

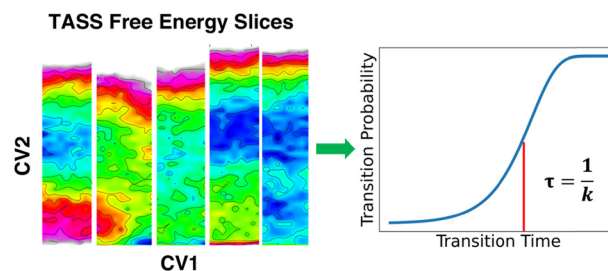
Raju Sardar, Soumili Dutta and Soumen Ghosh*



3721

Kinetics of barrier crossing events from temperature accelerated sliced sampling simulations

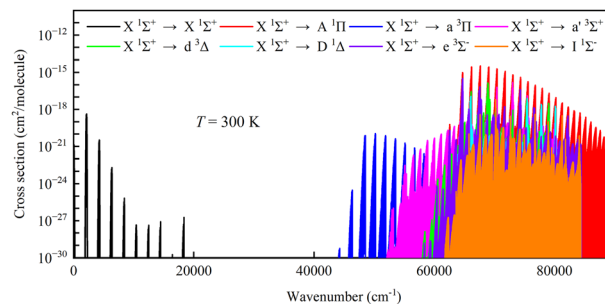
Sameer Saurav, Debjit Das, Ramsha Javed and Nisanth N. Nair*



3734

The rovibronic spectrum of carbon monoxide (CO) including its excited states

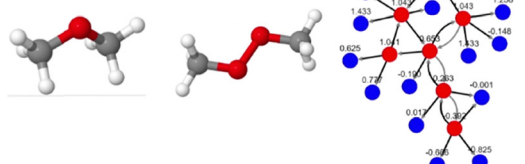
Shuai Zhang, Wei Chen* and Linhua Liu*



RESEARCH PAPERS

3743

Alchemical Space Exploration in Drug Design via Stochastic Expanding Boundary Optimization



Alchemical space exploration in drug design via stochastic expanding boundary optimization search

Konstantina Vaitis, Vasilios S. Melissas and Georgios C. Boulougouris*

CORRECTIONS

3759

Correction: Azothiophene-based molecular switches: influence of substituent position and solvent environment on photophysical behavior

Xin Zhang, Konstantinos T. Kotoulas, P. M. Anuththara Bandaranayake, Dilani Chathumalee, Nuha Ehsan, Patrick R. Huddleston, John D. Wallis and Carole C. Perry*

3760

Correction: De-transition-metallization of cathode materials for constructing high-performance solid-state electrolytes in potassium-ion batteries

Mengqi Wu, Meitong Liu, Xiangyu Yao, Chenyang Jing, Dongxiao Kan* and Ruqian Lian*

