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See Osamu Shirai *et al.*, pp. 3161–3167.
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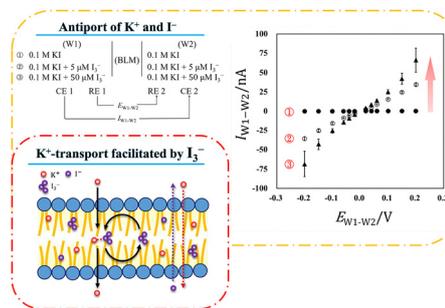
Inside cover
See Anne P. Rasmussen *et al.*, pp. 3168–3173.
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RESEARCH PAPERS

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

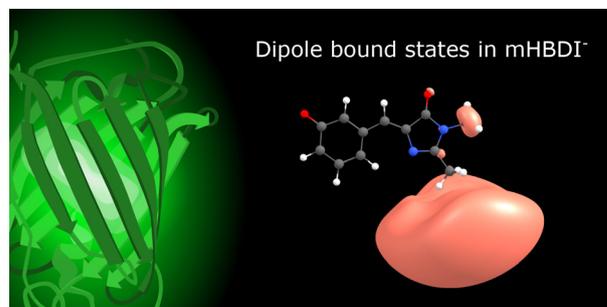
Weipai Chuang, Keisei Sowa, Yuki Kitazumi and Osamu Shirai*



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



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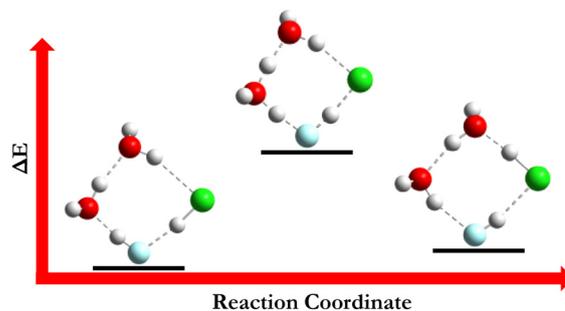
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Concerted proton transfer in homogeneous and heterogeneous cyclic hydrogen-bonded clusters of H₂O, HF, and HCl

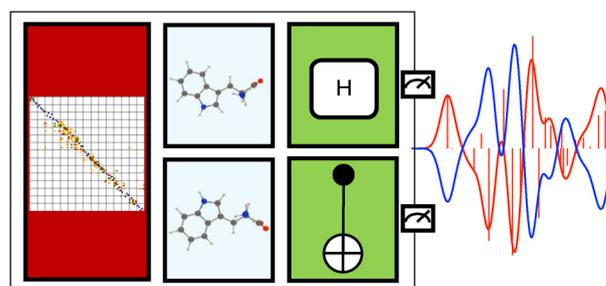
Max R. Tucker, Yuan Xue, Nathan R. Speake, Eden Nickolson, Jeremy M. Carr and Gregory S. Tschumper*



3183

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

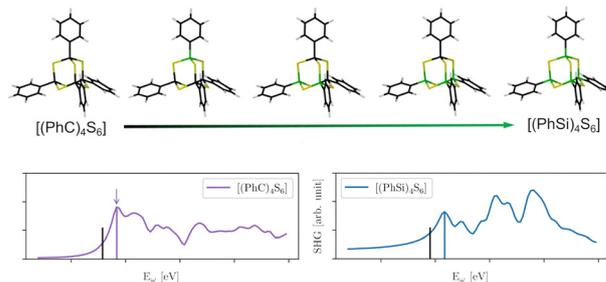
Renato Olarte Hernandez, Armand Soldera and Benoît Champagne*



3193

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

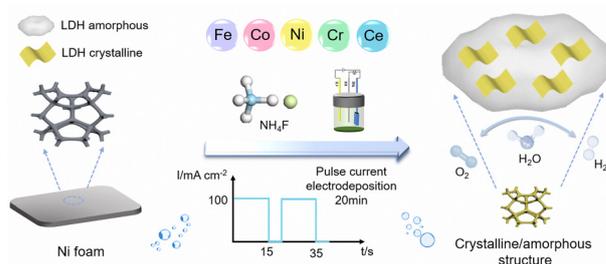
Ferdinand Ziese, Stefanie Dehnen and Simone Sanna



3204

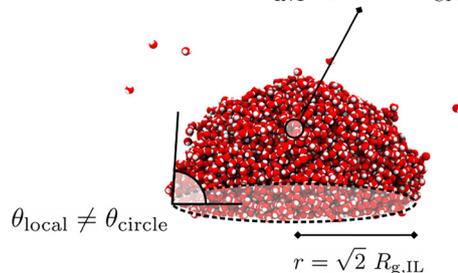
High-entropy FeCoNiCrCe layered double hydroxides by facile pulse current electrodeposition as high performance electrocatalysts for the oxygen evolution reaction

Xinyu Yang and Qianqiao Chen*



3213

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

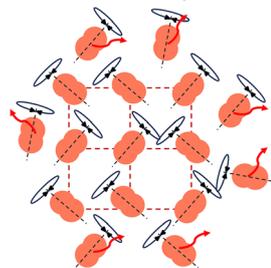


Robust methods for the characterization of droplet behavior in molecular dynamics: from contact radius to contact angle

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

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Heterogeneous translational dynamics
in core and surface regions



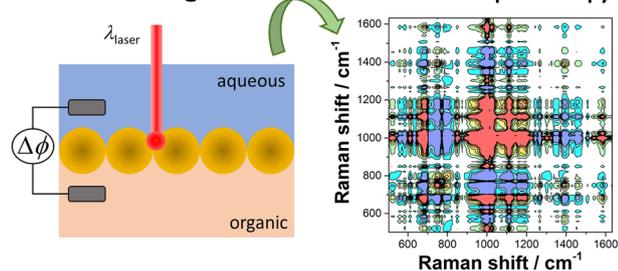
Heterogeneous translational dynamics of succinonitrile in the plastic crystalline phase

Keiko Nishikawa* and Kozo Fujii

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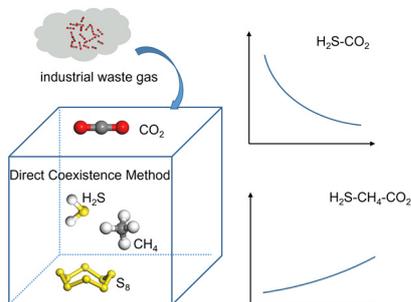
2D Correlation Spectroscopy



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*

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

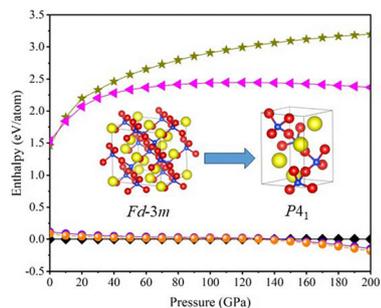
Shuangli Yue, Nong Li, Li Wang,* Ying Wan, Chengxin He, Li Zhang* and Mingli Yang



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

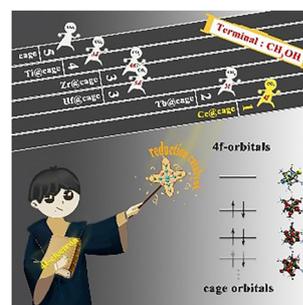
Kai Hu, Yixing Geng, Yanying Zhao, Yuqiu Gu,*
Jinqing Yu* and Xueqing Yan*



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

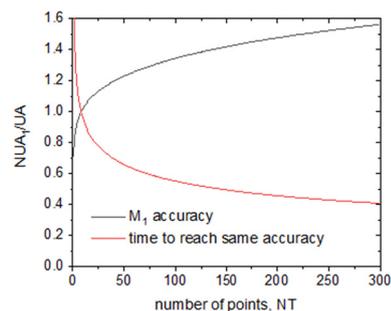
Zhiyuan Zhang, Jiarui Li, Pawel M. Kozlowski,
Wang Cong, Kamran Akbar, Yanning Zhang,*
Georg Schreckenbach,* Yang Gao* and Zhiming Wang



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Analytically optimized noise redistribution in pulsed dipolar EPR spectroscopy

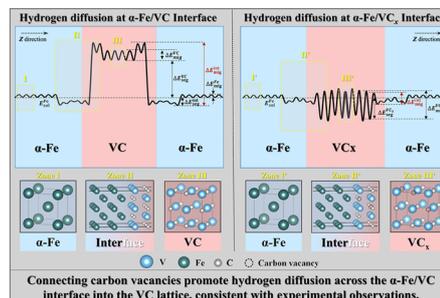
V. M. Nekrasov, A. G. Matveeva,* V. N. Sryamina,
S. A. Agarkin and M. K. Bowman



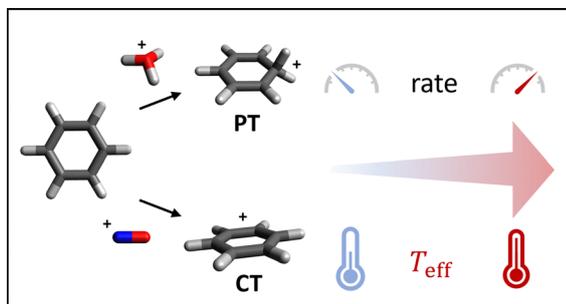
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Carbon vacancy network mediated hydrogen trapping at the α -Fe/VC interface

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



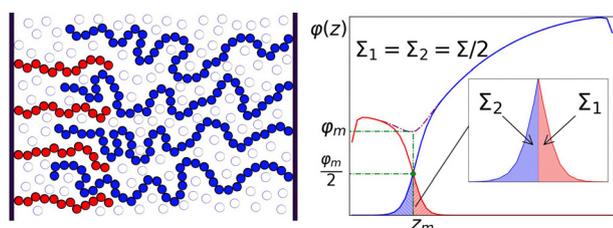
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Investigations on the field dependency of proton and charge transfer kinetics in atmospheric pressure corona discharge sources

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

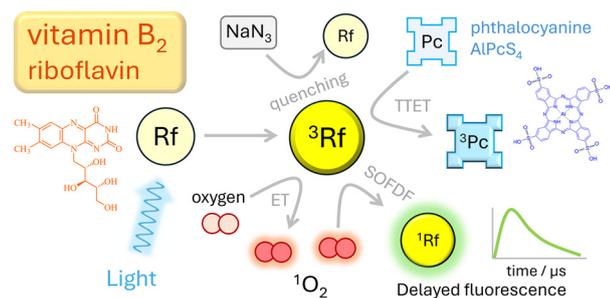
3305



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

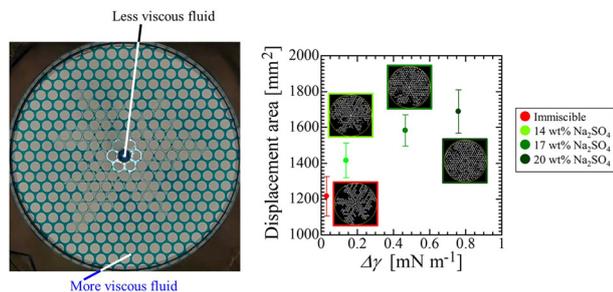
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Riboflavin – understanding the dynamics and interactions of the triplet state

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

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

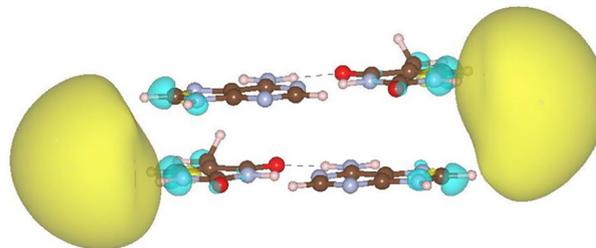
Shunta Kiuchi, Yuichiro Nagatsu, Takahiko Ban,
Manoranjan Mishra and Ryuta X. Suzuki*



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

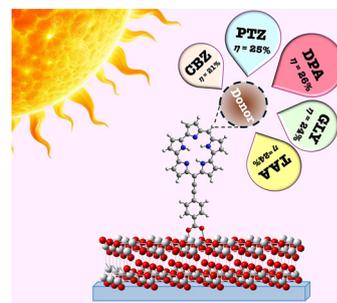
Raul Quintero-Monsebaiz, Per Hyldgaard and Elsebeth Schröder*



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

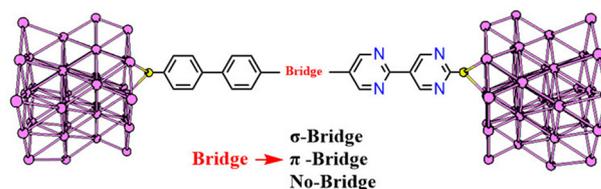
Swati Singh Rajput, Samarth Razdan, Tejendra Banana, Neelam Chandravanshi and Md Mehboob Alam*



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

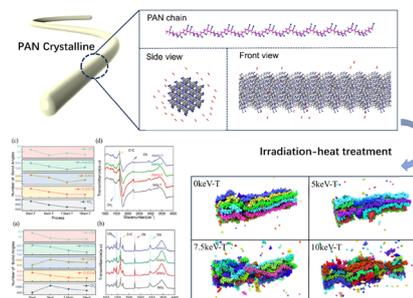
Morad M. El-Hendawy,* Hend S. Abd Elkhair and Mahmoud M. A. Mohamed



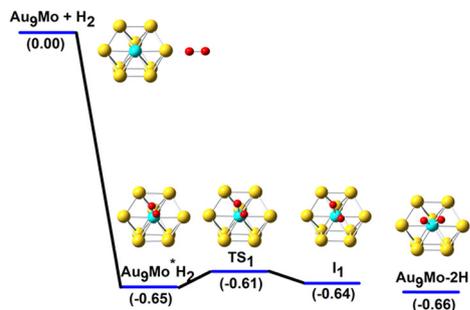
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Defect evolution and molecular transformation in the crystalline region of polyacrylonitrile fibers during irradiation-heat pre-oxidation: integrated simulation and experimental study

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



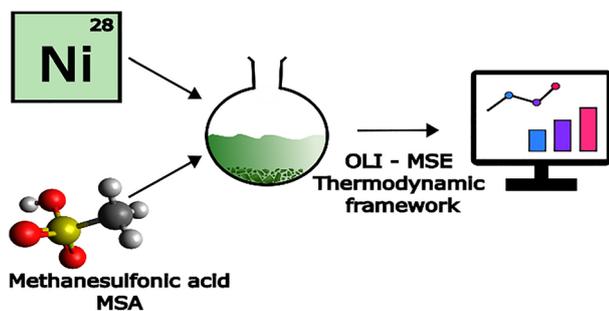
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DFT investigation of Au_nMo ($n = 2-12$) clusters: the barrierless hydrogen adsorption behavior of Au_9Mo

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

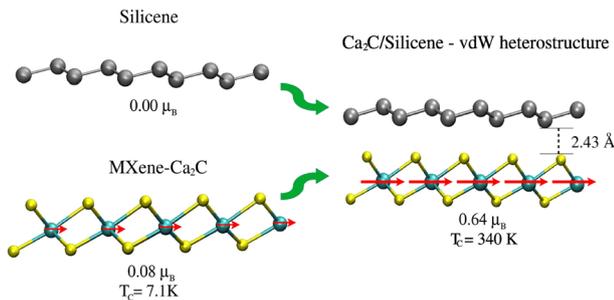
3401



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*

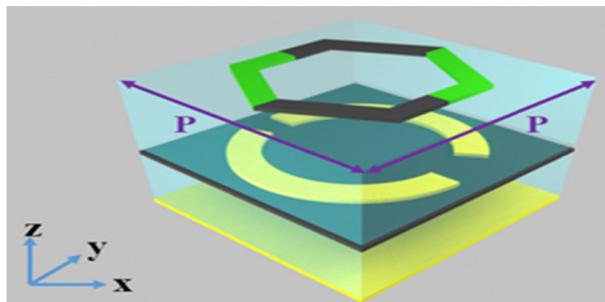
3415



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



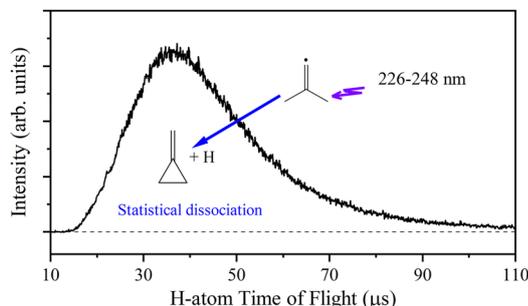
A dynamically reconfigurable terahertz metasurface enabled by hybrid $Ge_2Sb_2Te_5$ and VO_2 phase-change materials

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



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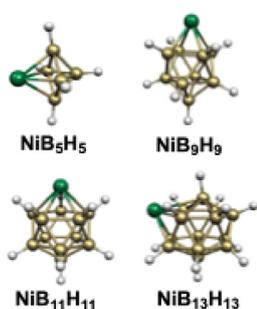
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H atom product channels in the ultraviolet photodissociation of the 2-methyl-1-propenyl radical

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

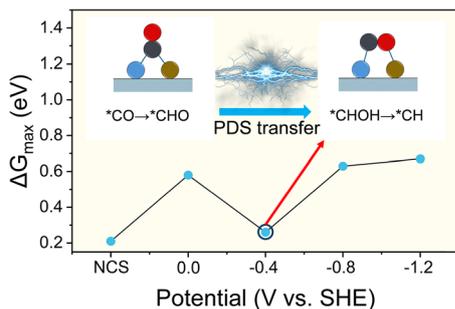
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Bare group 10 metal atoms as vertices in polyhedral metallaboranes: spherical aromaticity in the icosahedral MB₁₁H₁₁ systems

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

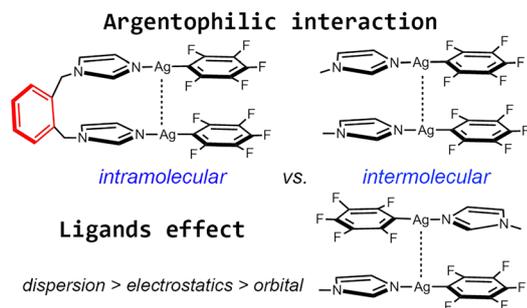
3501



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*

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

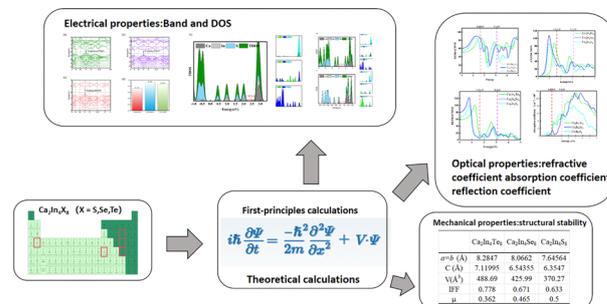
Yuan Xu,* Shan Liao and Peifeng Su



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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

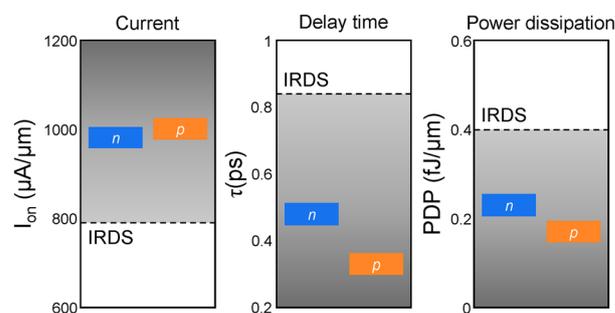
Wenbin Zhu, Beitong Cheng, Changcheng Chen,* Yue Cheng, Shuaikang Zhang, Kunzhuo Zhao, Zhengjun Wang, Xinhui Zhang, Chunling Zhang, Jiangzhou Xie, Yaxin Xu, Xiaoning Guan, Gang Liu* and Pengfei Lu*



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

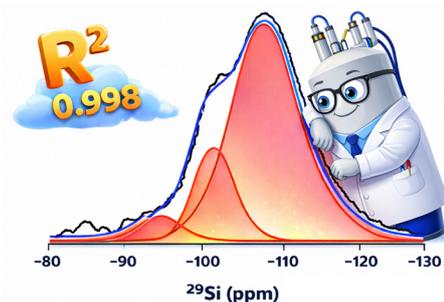
Hong Li,* Xiaotian Hu, Pengyang Liu, Fengbin Liu and Jing Lu*



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

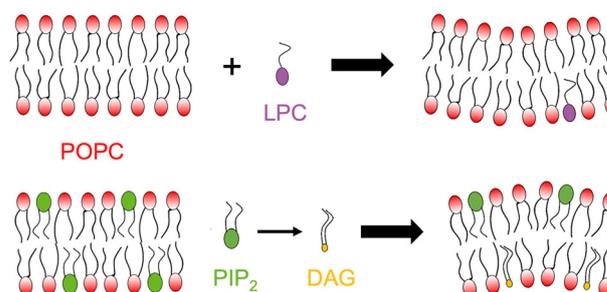
Valentina V. Sobornova and Ilya A. Khodov*



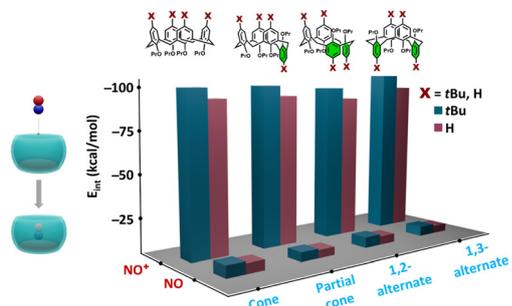
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Lipid bilayer membranes with asymmetrically distributed LPC and DAG

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



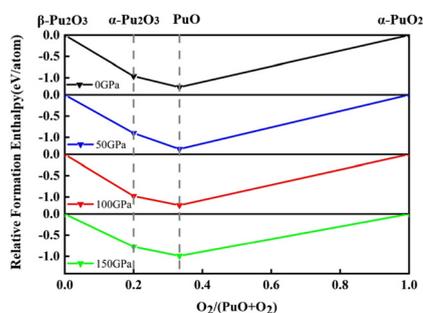
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Host–guest interaction of NO and NO⁺ species with calixerenes: dissecting the impact of conformational and confinement effects

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

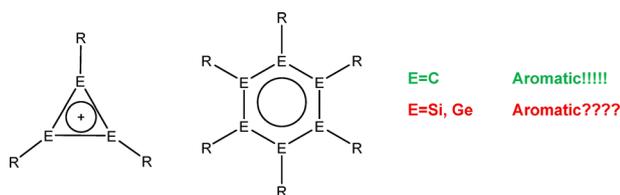
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High-pressure tuning of electronic structures, stability and mechanical properties of plutonium oxides: a DFT+U study

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

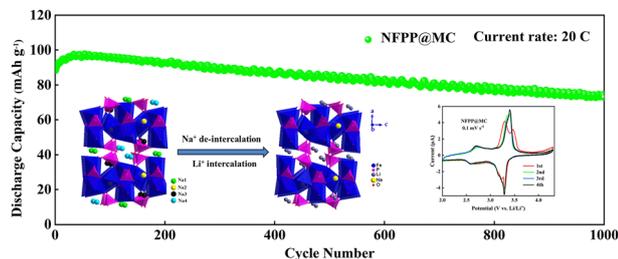
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The limit of the current aromaticity concept

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

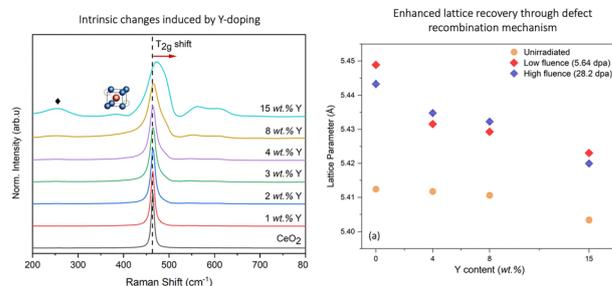
Zonghui Yi,* Hui Zhang, Zhiyuan Cheng, Lin Xie and Jiangping Cao



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

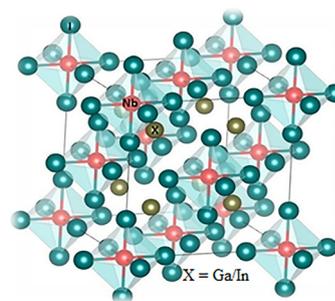
R. Mohun,* T. Cordara, J. McCloy, M. H. Weber, S. C. Middleburgh and C. L. Corkhill



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

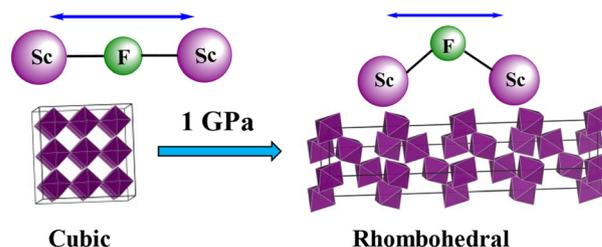
Afsar Ul Mulk, Malak Azmat Ali,* Jawad Hussain, Omar Alsalmi and Habib Ullah



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Anisotropic negative thermal expansion in high-pressure phases of ScF₃

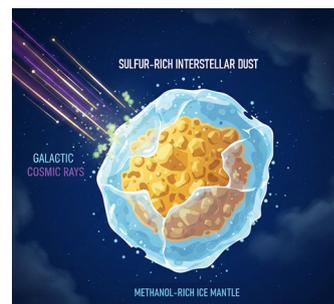
Soumya Mondal, Shovan Das and Ayan Datta*



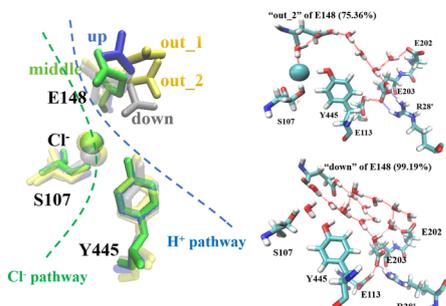
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Irradiation of methanol ice on a sulfur-rich dust analogue at 25 K: a mid-infrared spectroscopic study

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*



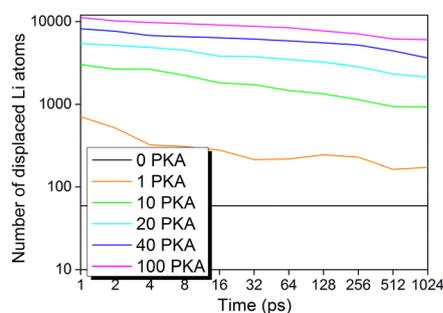
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Molecular dynamics investigation of the interaction between central-site chloride binding and proton transport in EcCLC

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

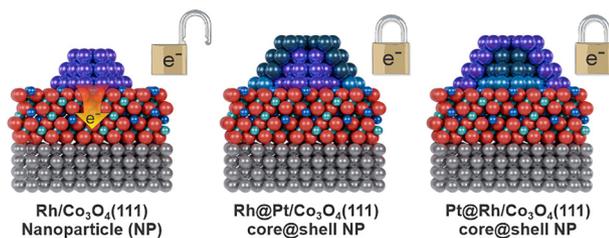
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Disorder and damage recovery in irradiated lithium oxide

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

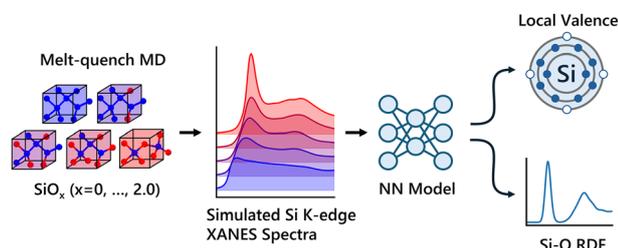
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A bimetallic strategy to modulate electronic metal support interaction in Co₃O₄(111)-based catalysts: the case of supported Rh–Pt core–shell nanoparticles

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

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

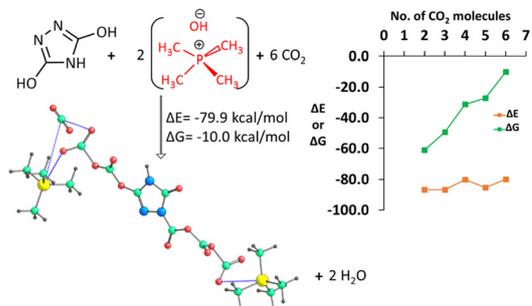
Yu Fujikata,* Hiroki Sugisawa and Teruyasu Mizoguchi



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

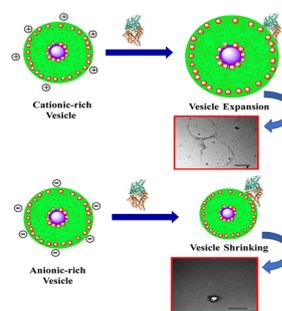
Puthiyavalappil K. Arathi, D. Sudha and Cherumuttathu H. Suresh*



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

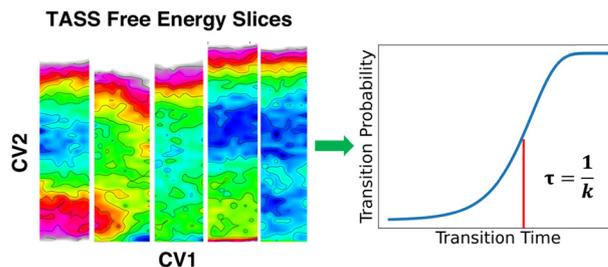
Raju Sardar, Soumili Dutta and Soumen Ghosh*



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Kinetics of barrier crossing events from temperature accelerated sliced sampling simulations

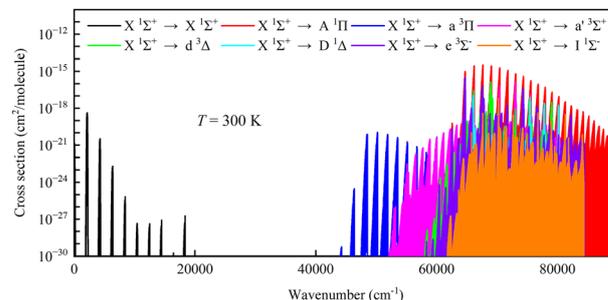
Sameer Saurav, Debjit Das, Ramsha Javed and Nisanth N. Nair*



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

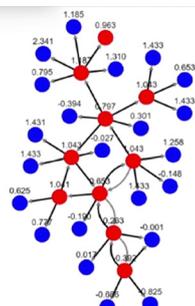
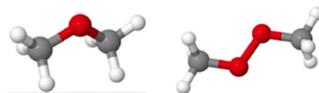
Shuai Zhang, Wei Chen* and Linhua Liu*



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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

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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*

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

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