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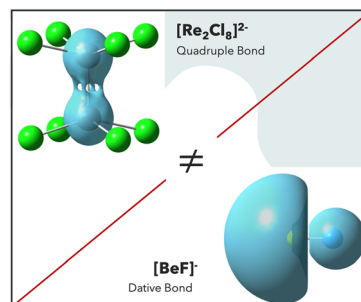
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2333

Exploring the bonding in alkaline earth halides AeX^- ($\text{Ae} = \text{Be}-\text{Ba}$, $\text{X} = \text{F}-\text{I}$) from Fermi hole localization and QTAIM perspectives

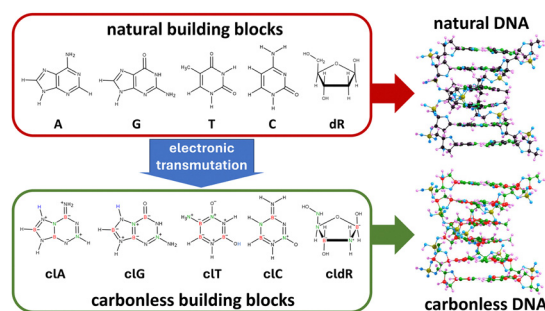
Luis Rincon, Valeria Bedoya, Luis E. Seijas, Vladimir Rodríguez, Cesar Zambrano and F. Javier Torres*



2343

Carbonless DNA

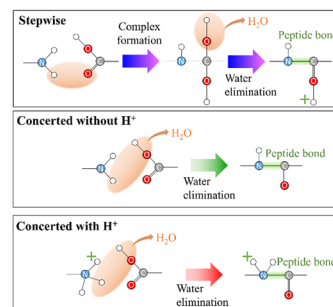
Piotr Skurski* and Jakub Brzeski



2363

On peptide bond formation from protonated glycine dimers in the gas phase: computational insight into the role of protonation

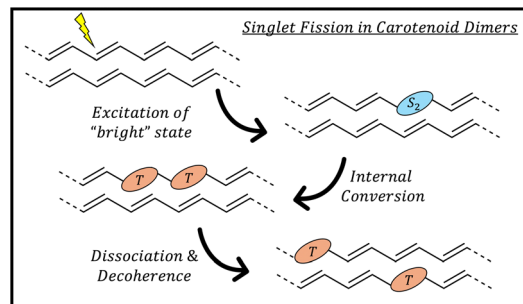
Léo Lavy, Denis Comte, Florent Calvo, Bernadette Farizon, Michel Farizon* and Tilmann D. Märk



2371

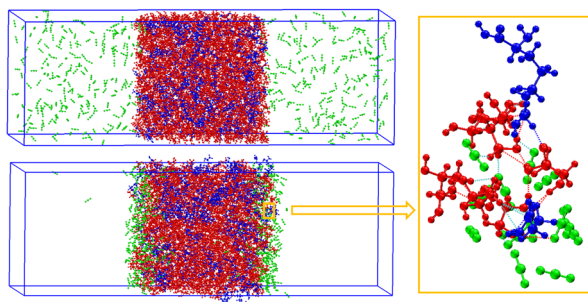
Singlet fission in carotenoid dimers – the role of the exchange and dipolar interactions

Alexandru G. Ichert* and William Barford*



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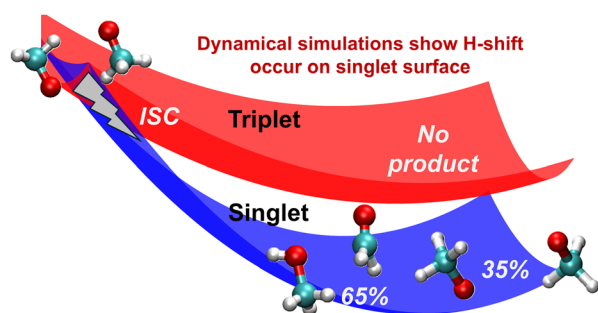
2381



CO₂ adsorption in natural deep eutectic solvents: insights from quantum mechanics and molecular dynamics

Chengxu Zhu, Hannah Wood, Paola Carbone, Carmine D'Agostino* and Sam P. de Visser*

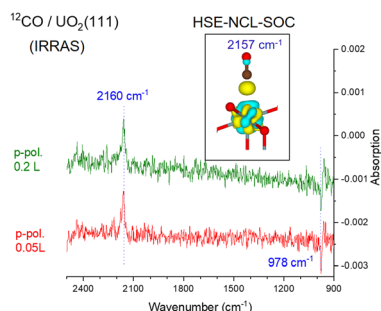
2395



Dynamics of hydrogen shift reactions between peroxy radicals

Imon Mandal, Christopher David Daub, Rashid Valiev, Theo Kurtén* and R. Benny Gerber*

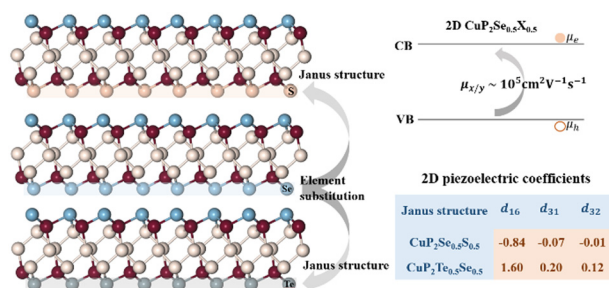
2405



Exploring molecule–surface interactions of urania via IR spectroscopy and density functional theory

Hicham Idriss,* Maria Andrea Barral, Solange Mariel Di Napoli, Gustavo E. Murgida, Eric Sauter, Ana María Llois, M. Verónica Ganduglia-Pirovano, Verónica Laura Vildosola* and Christof Wöll

2418



Ultrahigh carrier mobility and multidirectional piezoelectricity in 2D Janus copper-containing chalcogenide monolayers

Mengbing Liu, Xingxu Meng, Yuli Yan and Huabing Yin*

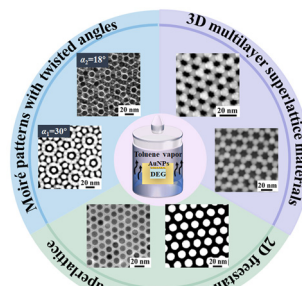


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Templated self-organization of polymer-tethered gold nanoparticles into freestanding superlattices at the liquid–air interface

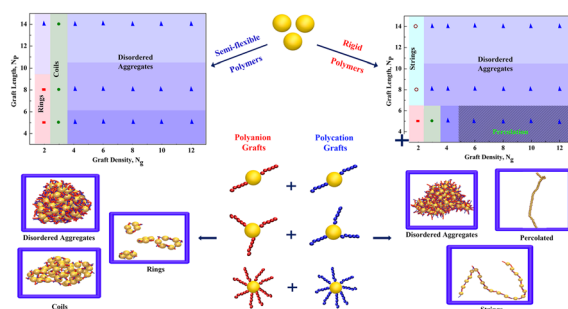
Ye Gao, Lingli Wan, Yuqing Song, Shan Gao, Nan Yan,*
Fan Wu* and Yanqiu Du*



2434

Role of polymer graft stiffness in electrostatic-driven self-assembly of nanoparticles in solutions

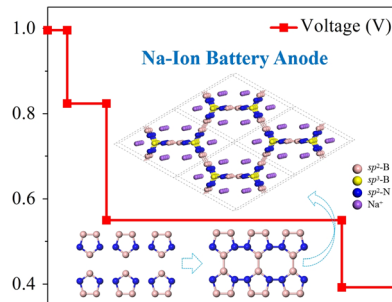
Rajesh Pavan Pothukuchi* and Mithun Radhakrishna



2444

A new 3D metallic, ductile, and porous boron nitride as a promising anode material for sodium-ion batteries

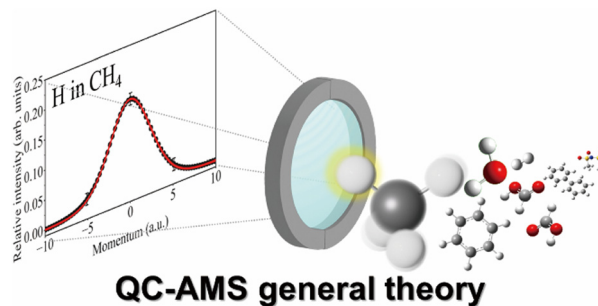
Wei Sun, Qian Wang* and Puru Jena



2453

Theoretical atomic momentum spectroscopy of diatomic, triatomic and polyatomic molecules

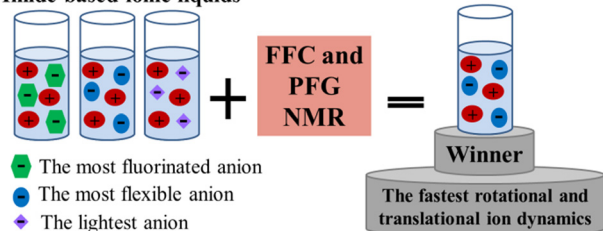
Satoru Kanaya, Yuuki Onitsuka, Noboru Watanabe,
Hirohiko Kono and Masahiko Takahashi*



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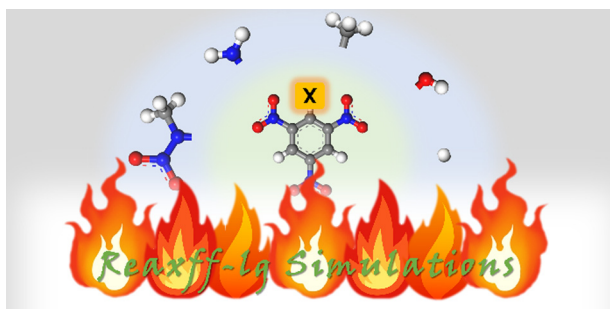
Imide-based ionic liquids



Dynamics of fluorinated imide-based ionic liquids using nuclear magnetic resonance techniques

Tawhid Pranto, Carla C. Fraenza,* Frederik Philippi, Daniel Rauber, Christopher W. M. Kay, Tom Welton, Steven G. Greenbaum and Sophia Suarez*

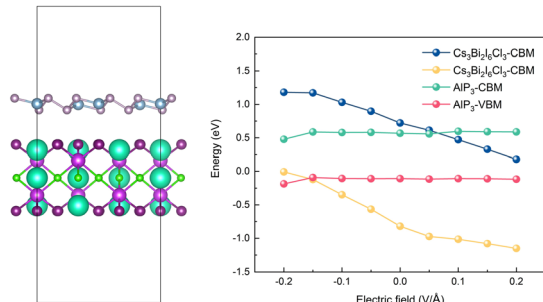
2473



The substituent effect on the heat-induced pyrolysis mechanism of energetic materials: a case of reactive molecular dynamics simulations on nitrobenzene compounds

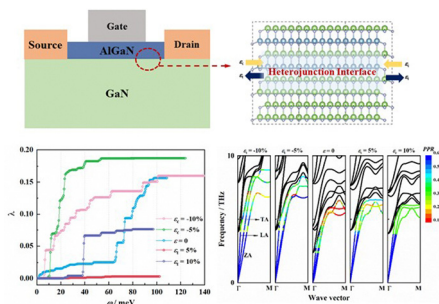
Shuangfei Zhu,* Chaowen Yang, Shufen Zheng, Shuhai Zhang, Yahong Chen and Yang Liu

2485

The tunable electronic band structure of a $\text{AlP}_3/\text{Cs}_3\text{Bi}_2\text{I}_6\text{Cl}_3$ van der Waals heterostructure induced by an electric field: a first-principles study

Cheng-sheng Liao, Lin Lang, Qiu-yi Wang, Yu-qing Zhao and Zhuo-liang Yu*

2495



Electron–phonon coupling and thermal transport properties of GaN/AlGaIn heterojunction under strain regulation

Jiao Chen, Zumeng Shan, Baoyi Hu, Zhaoliang Wang,* Dawei Tang and Ke Xu

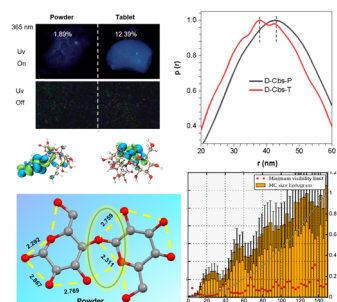


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Elucidating the mechanism behind the significant changes in photoluminescence behavior after powder compression into a tablet

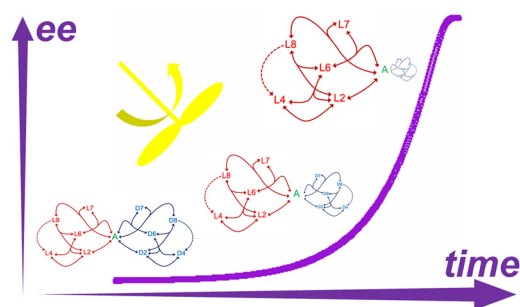
Xiaoping Lei, Qingfeng Wu, Xiangxi Zhang, Qing Zhou* and Lingmin Yi*



2516

Viedma deracemization mechanisms in self-assembly processes

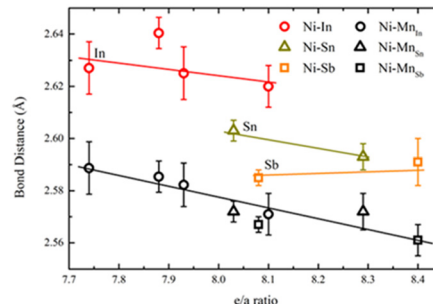
Josep M. Ribó, David Hochberg,* Thomas Buhse and Jean-Claude Micheau



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Role of local structural distortions in the variation of martensitic transformation temperature with e/a ratio in $\text{Ni}_2\text{Mn}_{1+x}\text{Z}_{1-x}$ ($\text{Z} = \text{In, Sn or Sb}$) alloys

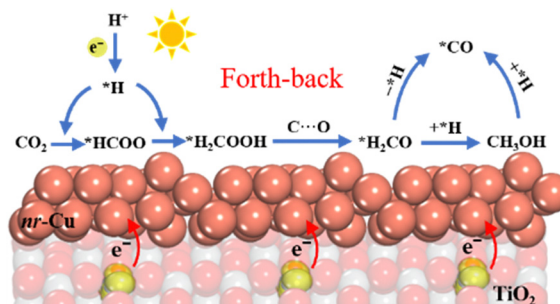
Nafea Manea, Edmund Welter and K. R. Priolkar*



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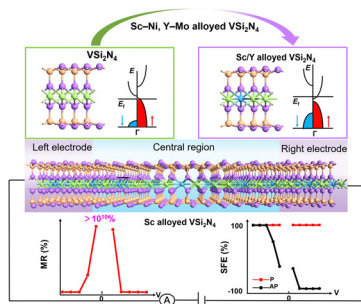
Insight into photocatalytic CO_2 reduction on TiO_2 -supported Cu nanorods: a DFT study on the reaction mechanism and selectivity

Ying Liu, Jinyang Zhang, Jiamin Jin, Huihui Liu, Guanhua Ren, Peijun Hu* and Haifeng Wang*



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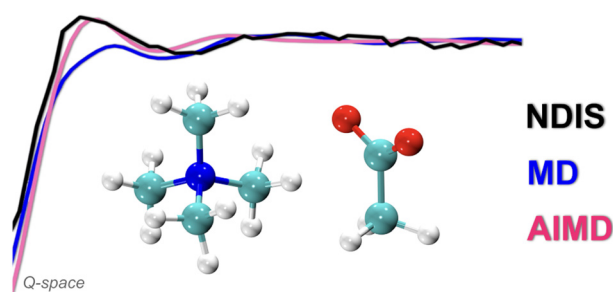
2545



Alloying two-dimensional VSi_2N_4 to realize an ideal half-metal towards spintronic applications

Jin-Lan Sun, Wei-Kang Zhang, Mi-Mi Dong,
Zong-Liang Li, Chuan-Kui Wang* and Xiao-Xiao Fu*

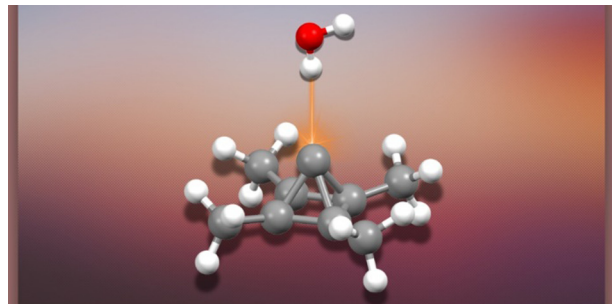
2553



Ion pairing in aqueous tetramethylammonium–acetate solutions by neutron scattering and molecular dynamics simulations

Ngoc Lan Le Nguyen, Ondrej Tichacek, Pavel Jungwirth,
Hector Martinez-Seara, Philip E. Mason* and
Elise Duboué-Dijon*

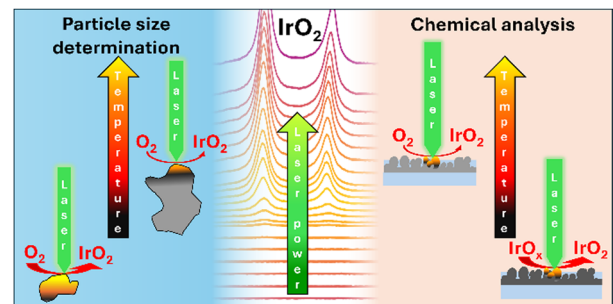
2563



Evidence of strong $\text{O–H}\cdots\text{C}$ interactions involving apical pyramidane carbon atoms as hydrogen atom acceptors

Ivana S. Veljković, Miroslavka Malinić and
Dušan Ž. Veljković*

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Laser induced oxidation Raman spectroscopy as an analysis tool for iridium-based oxygen evolution catalysts

Sebastian Speer, Sven Jovanovic,* Alexandre Merlen,
Francesco Bartoli, Kiran Kiran, Niklas Wolf, André Karl,
Eva Jodat and Rüdiger-A. Eichel

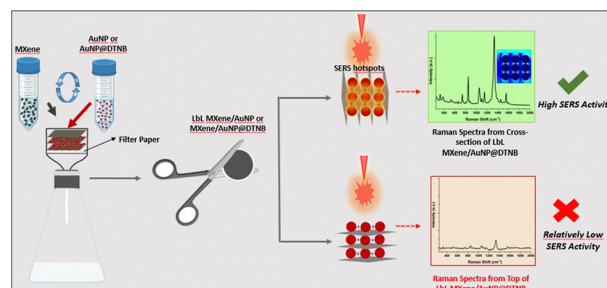


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Layer-by-layer thin films of Ti_3C_2 MXene and gold nanoparticles as an ideal SERS platform

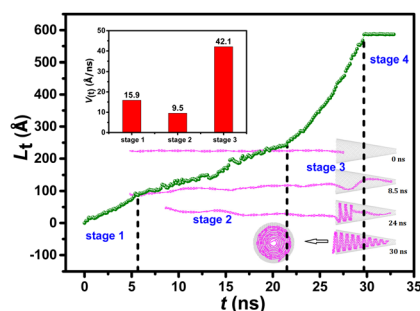
Hayrunnisa Mazlumoglu and Mehmet Yilmaz*



2588

Constructing conical helices inside carbon nanocones

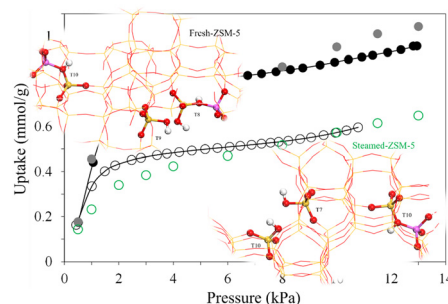
Yuliang Yin, Qinzhen Yu, Hongjin Fu and Yunfang Li*



2601

A complementary experimental and computational study on methanol adsorption isotherms of H-ZSM-5

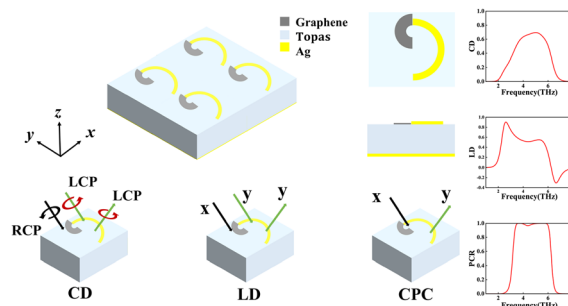
Santhosh K. Matam,* Lotfi Boudjema, Matthew G. Quesne, James D. Taylor and C. Richard A. Catlow



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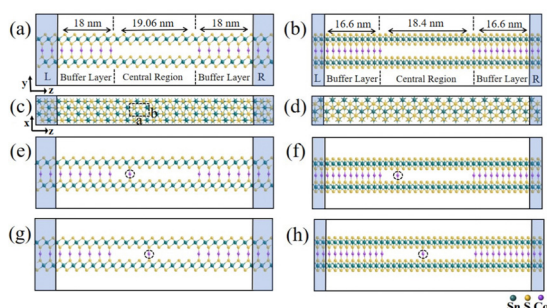
Design of a graphene-based chiral trifunctional tunable terahertz metasurface

Kun Hu, Yunpeng Yao, Lipengan Ye, Zongli Hu, Bin Tang and Wei Su*



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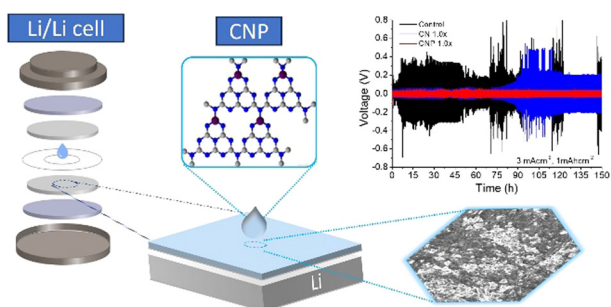
2623



Effect of defects on ballistic transport in a bilayer SnS_2 -based junction with Co intercalated electrodes

Miao Liu, Huan Wang,* Xiaojie Liu,* Yin Wang* and Haitao Yin*

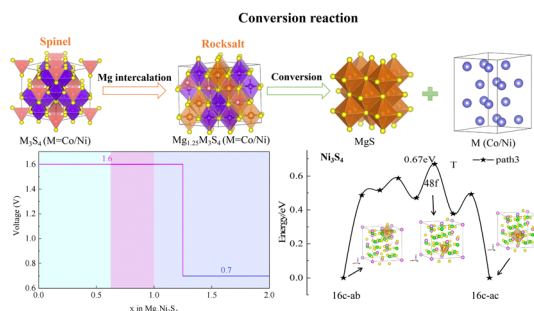
2631



2D P-doped carbon nitride as an effective artificial solid electrolyte interphase for the protection of Li anodes

Franco Eroles, Yesica Celeste Villagrán López, María Beatriz López, Martin E. Zoloff Michoff,* Guillermina Luque and Fernando Cometto*

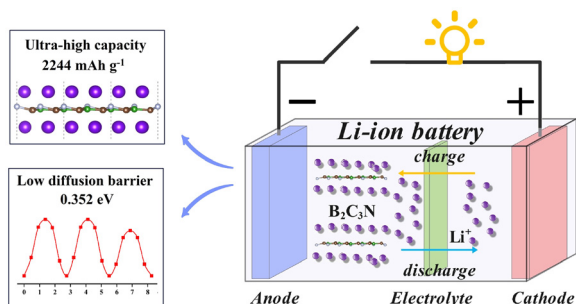
2644



Unraveling the conversion mechanism toward spinel sulfides as cathode materials for Mg-ion batteries

Jinming Pan, Danmei Gao, Jianxian Qiao, Yuping Liu,* Jing Xu,* Bo Shang, Changguo Chen,* Guangsheng Huang, Dingfei Zhang and Fusheng Pan

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$\text{B}_2\text{C}_3\text{N}$ monolayers with high theoretical capacity as anode materials for lithium-ion batteries: first-principles calculations

Yutong Zou, Yaqi She, Liuxu Zhao, Ailing Liu, Bo Sun, Yuhong Jiang, Chunlei Kou,* Miao Zhang* and Yuanye Tian*

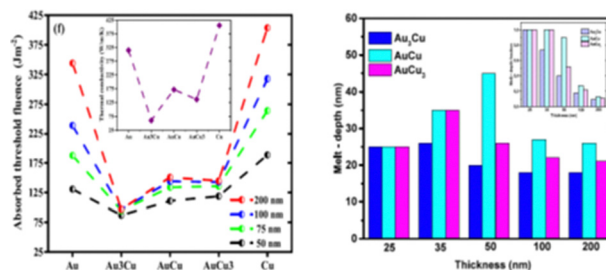


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Enhanced two-temperature model and its application in comprehensive analysis of femtosecond laser melting of gold, copper and their alloys

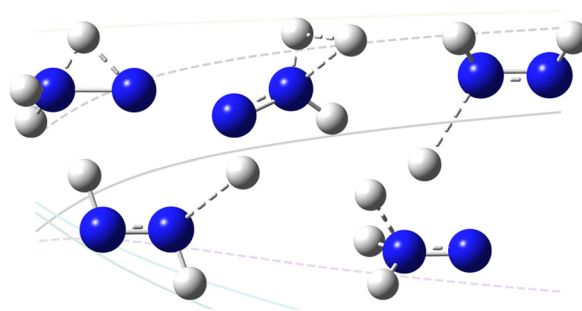
Aeaby C. D.* and Aditi Ray



2680

Pressure-dependent kinetic analysis of the N_2H_3 potential energy surface

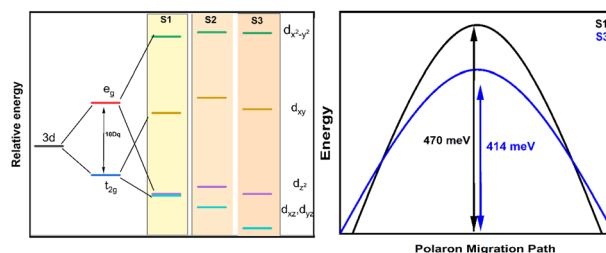
Michal Keslin, Kfir Kaplan and Alon Grinberg Dana*



2692

Effect of strain on the electronic structure and polaronic conductivity of $LiFePO_4$

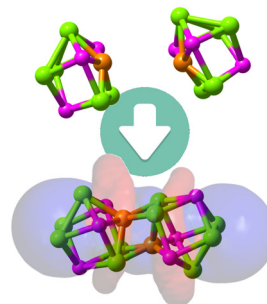
Manisha, Mukul Gupta, V. Raghavendra Reddy and Sevi Murugavel*



2704

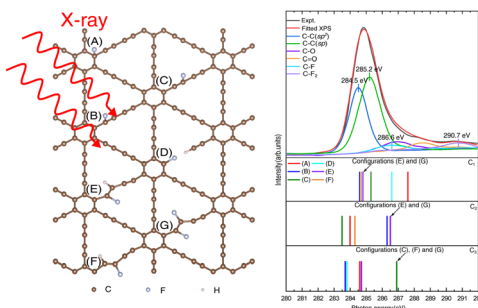
$[CuSn_5Sb_3]_2^{4-}$ as a dual spherical–spherical aromatic heterometallic cluster bridged via an antiaromatic Cu_2Sn_2 motif

Peter L. Rodríguez-Kessler and Alvaro Muñoz-Castro*



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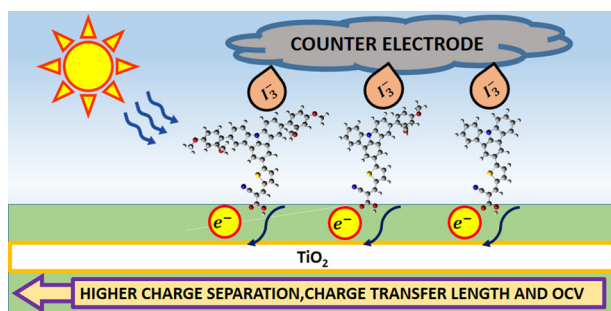
2711



Towards sensitive identification of fluorinated graphdiyne configurations by computational X-ray spectroscopy

Hai-Bo Li, Xiu-Neng Song, Chuan-Kui Wang, Weijie Hua and Yong Ma*

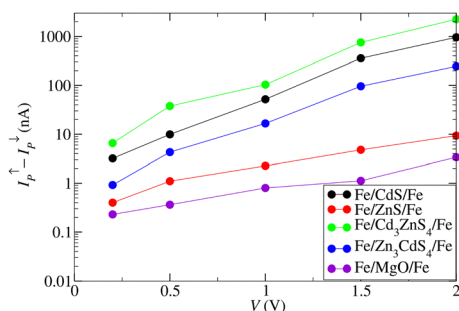
2720



A study on indolo[3,2,1-jk]carbazole donor-based dye-sensitized solar cells and effects from addition of auxiliary donors

Harkishan Dua, Debolina Paul and Utpal Sarkar*

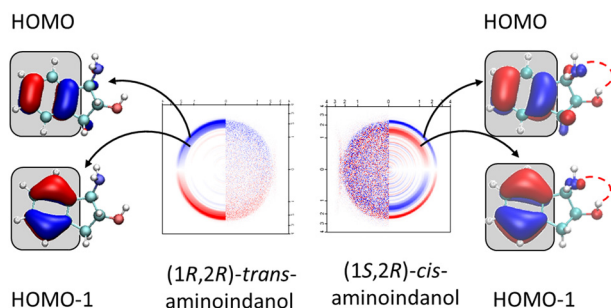
2732



Tunnel barriers for Fe-based spin valves providing high spin-polarized current

Gokaran Shukla, Hasan M. Abdullah and Udo Schwingenschlögl*

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The role of intramolecular hydrogen bonding in photoelectron circular dichroism: the diastereoisomers of 1-amino-2-indanol

Etienne Rouquet, Jennifer Dupont, Julien Vincent, Valéria Lepère, Anne Zehnacker,* Sebastian Hartweg, Gustavo A. Garcia and Laurent Nahon*

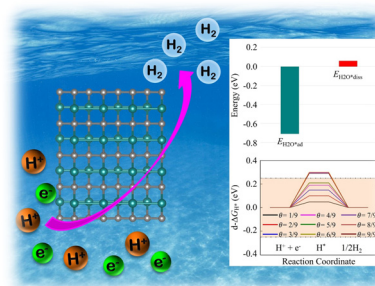


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Metallic PtC monolayer as a promising hydrogen evolution electrocatalyst

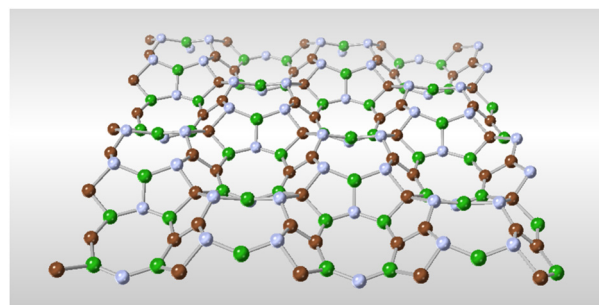
Huan Lou* and Chi Ma



2758

Promising mechanical, electronic and piezoelectric properties of grapheneplus-like BCN monolayer: insights from first-principles

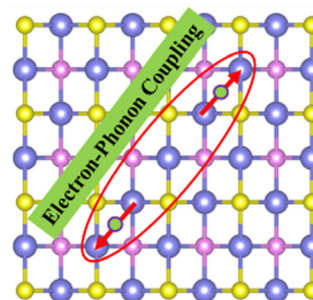
Jinyuan Liu, Yi Ding* and Yanli Wang*



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Emergent superconductivity driven by Van Hove singularity in a Janus Mo₂PS monolayer

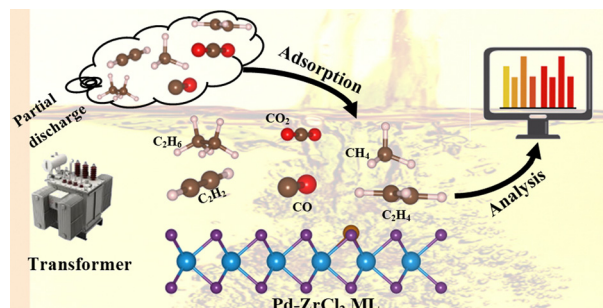
Meng Tang, Wenyuan Zhang, Guochun Yang* and Huiqiu Deng*



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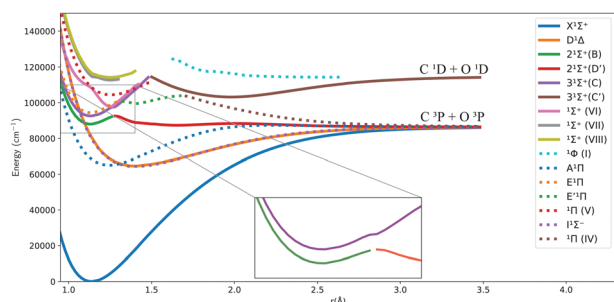
DFT study of Pd-doped ZrCl₂: a promising solution for dissolved gas molecule analysis in transformer oil

Yashasvi Naik, Disha Mehta, H. R. Mahida, Riddhi Desai and P. B. Thakor*



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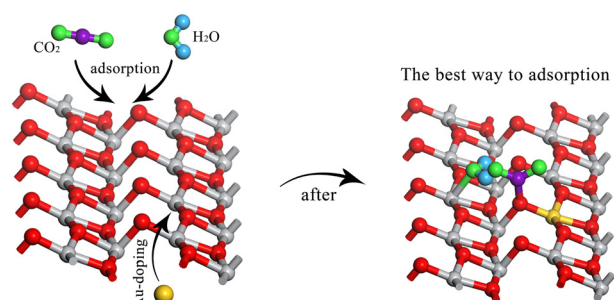
2783



Theoretical investigation of the $A^1\Pi-X^1\Sigma^+$, $B^1\Sigma^+-X^1\Sigma^+$, $C^1\Sigma^+-X^1\Sigma^+$, and $E^1\Pi-X^1\Sigma^+$ transitions of the CO molecule

Malathe Khalil, Salman Mahmoud, Ryan P. Brady, Mubarak Almehairbi, Marko Gacesa, Sergei N. Yurchenko, Jonathan Tennyson,* Amal Al Ghaferi and Nayla El-Kork*

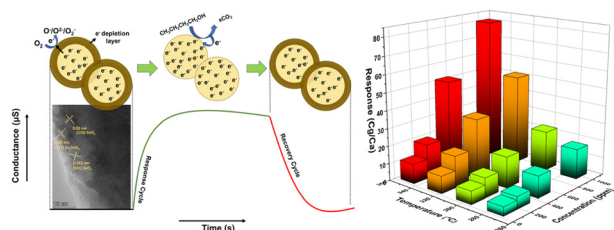
2802



First-principles study of CO₂ and H₂O adsorption on the anatase TiO₂(101) surface: effect of Au doping

Huan Zhang, Meijun Yin, Shuangli Du,* Yitao Li, Jialiang Bai, Haonan Chai, Jun Ren and Mingji Ding

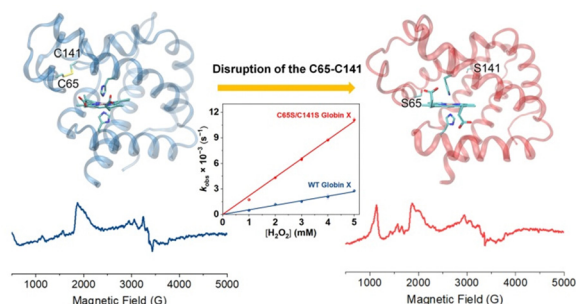
2817



Sensing of *n*-butanol vapours using an oxygen vacancy-enriched Zn₂SnO₄-SnO₂ hybrid-composite

Reshmi Thekke Parayil, Snehangshu Paine, K. Mukherjee,* D. Tyagi, Manoj Mohapatra and Santosh K. Gupta*

2828



Disruption of a potential disulfide bond of Cys65-Cys141 on the structure and stability of globin X from zebrafish

Aiqun Pan, Xichun Liu,* Hui Han, Shu-Qin Gao and Ying-Wu Lin*

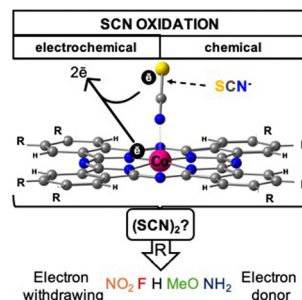


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Computational exploration of the electrochemical oxidation mechanism of thiocyanate catalyzed by cobalt-phthalocyanines

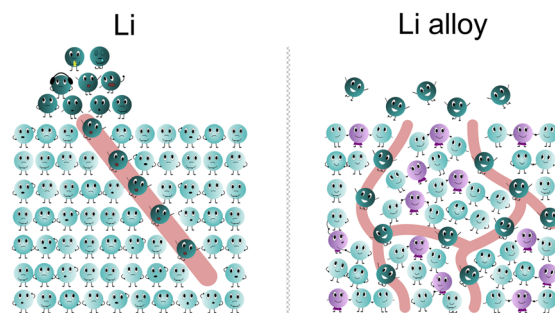
Sebastián Miranda-Rojas,* Néstor Gutiérrez-Sánchez, Carlos Orellana, Kevin Blanco-Esparguez, Sasha Gazzari-Jara, Paulina Sierra-Rosales and Fernando Mendizábal*



2845

Whisker-free lithium electrodeposition by tuning electrode microstructure

Alexey A. Rulev,* Yevgeniya O. Kondratyeva, Lada V. Yashina, Ilia P. Ivanenko and Daniil M. Itkis



CORRECTION

2852

Correction: *Ab initio* study of temperature-dependent piezoelectric and electronic properties of thermally stable GaPO₄

Xiaoqing Yang, Pan Guo, Shunbo Hu, Zhibin Gao, Wenliang Yao, Jinrong Cheng, Samuel Poncé, Baigeng Wang and Wei Ren*

