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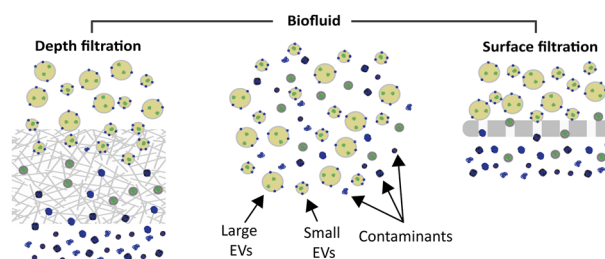
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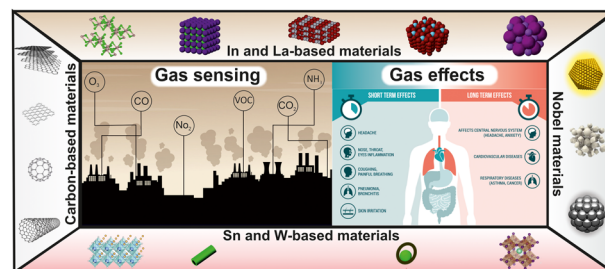
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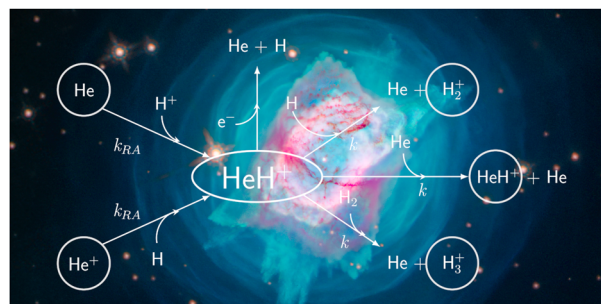


## PERSPECTIVES

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## The role of small molecular cations in the chemical flow of the interstellar environments

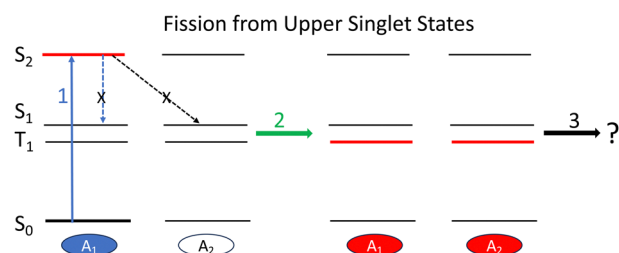
Lola González-Sánchez,\* N. Sathyamurthy and Francesco A. Gianturco



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Ronald P. Steer

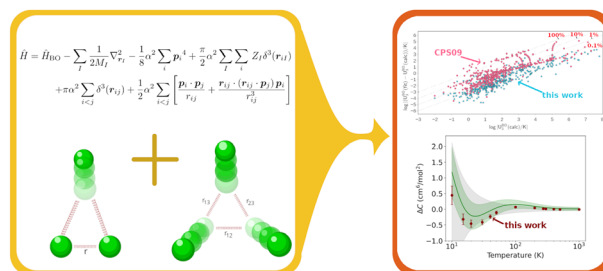


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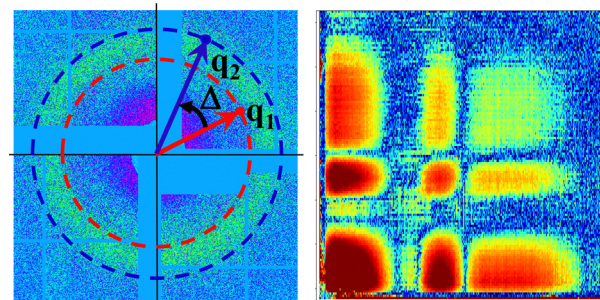
Jakub Lang,\* Giovanni Garberoglio, Michał Przybytek, Małgorzata Jeziorska and Bogumił Jeziorski



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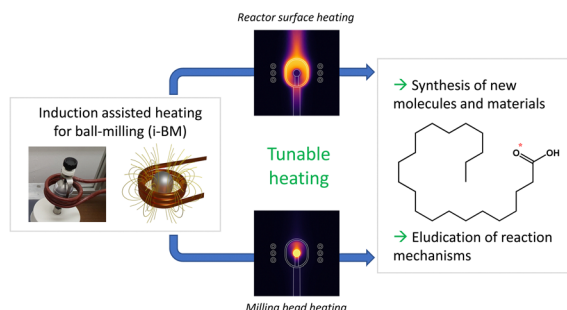
## Exploring fingerprints of ultrafast structural dynamics in molecular solutions with an X-ray laser

Ruslan P. Kurta,\* Tim B. van Driel, Asmus O. Dohn, Tim B. Berberich, Silke Nelson, Ivan A. Zaluzhnyy, Nastasia Mukharamova, Dmitry Lapkin, Diana B. Zederkof, Matthew Seaberg, Kasper S. Pedersen, Kasper S. Kjær, Geoffery Ian Rippey, Elisa Biasin, Klaus B. Møller, Luca Gelisio, Kristoffer Haldrup, Ivan A. Vartanyants and Martin M. Nielsen\*



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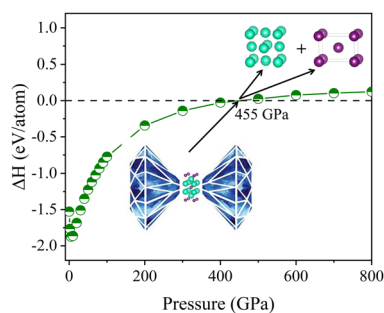
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### Induction-heated ball-milling: a promising asset for mechanochemical reactions

Gautier Félix,\* Nicolas Fabregue, César Leroy, Thomas-Xavier Métro, Chia-Hsin Chen and Danielle Laurencin\*

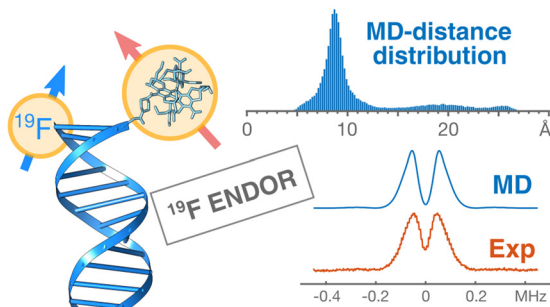
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Yanlei Geng, Jianfu Li,\* Zhaobin Zhang, Yang Lv, Zhenzhen Xu, Yong Liu, Jianan Yuan, Qinglin Wang and Xiaoli Wang\*

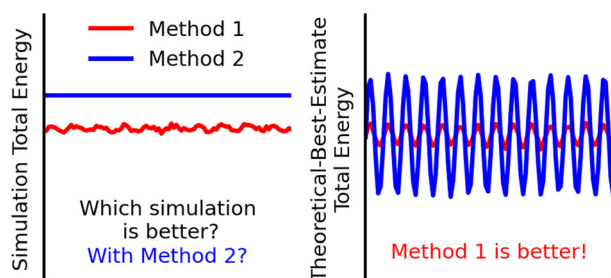
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### Energy-conserving molecular dynamics is not energy conserving

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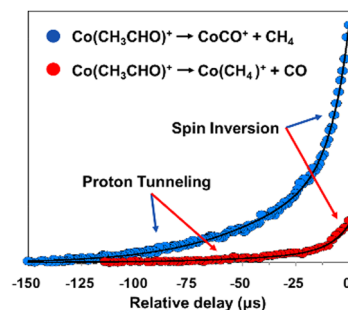


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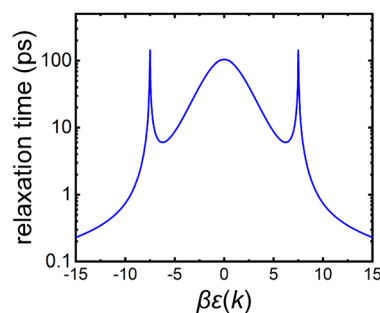
Tucker W. R. Lewis, Evan M. Mastin, Zachry C. Theis, Simon U. Okafor, Michael G. Gutierrez and Darrin J. Bellert\*



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## Carrier mobility of two-dimensional Dirac materials: the influence of optical phonon scattering

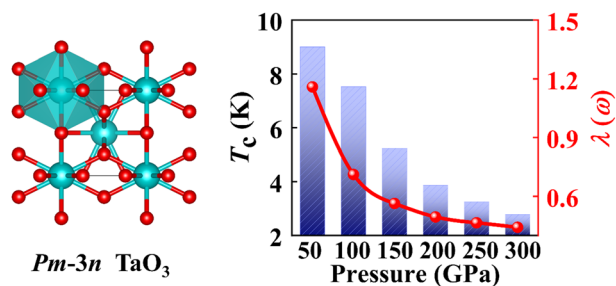
Yingqi Wang, Zijian Wang, Ting Cheng and Zhirong Liu\*



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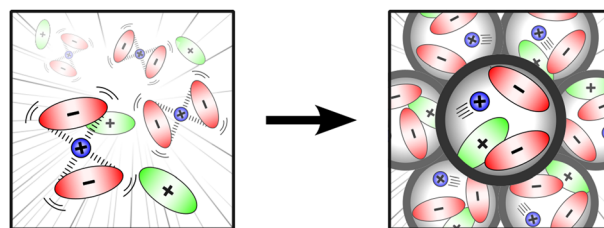
Wenjing Li, Xing Li, Xiaohua Zhang, Hong Yu, Fanjunjie Han, Aitor Bergara,\* Jianyan Lin,\* Jinhui Wu and Guochun Yang\*



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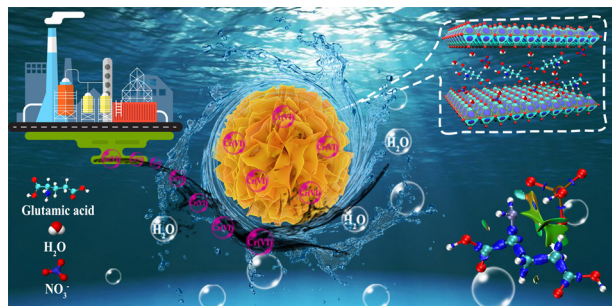
## Confinement-enhanced $\text{Li}^+$ ion dynamics in an ionic liquid-based electrolyte in porous material

Janis Hessling, Martin Lange and Monika Schönhoff\*



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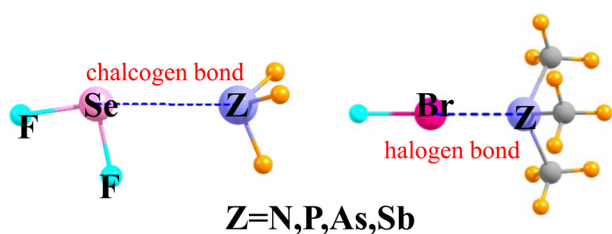
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### Unveiling glutamic acid-functionalized LDHs: understanding the Cr(VI) removal mechanism from microscopic and macroscopic view points

Xianyong Hong, Mingxing Shi, Zhoutian Ding, Chao Ding, Ping Du, Mingzhu Xia\* and Fengyun Wang\*

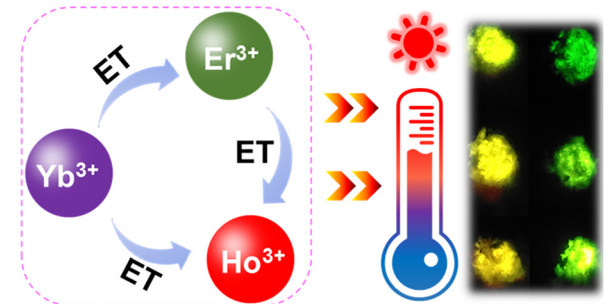
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### Heavy pnictogen atoms as electron donors in sigma-hole bonds

Akhtam Amonov and Steve Scheiner\*

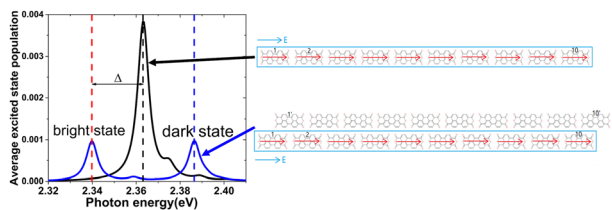
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### Manipulating the thermometric behaviors of Er<sup>3+</sup>/Yb<sup>3+</sup>/Ho<sup>3+</sup>-tridoped La<sub>2</sub>Mo<sub>3</sub>O<sub>12</sub> polychromatic upconverting microparticles via adjusting spatial mode and a sensing strategy

Huocheng Lv, Xiaoqing Lai, Weiping Li, Laihui Luo\* and Peng Du\*

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### Optical response and multi-exciton effects in 2D PTCDA aggregates with local excitation

An Wei, Deyin Fang, Siyuan Lyu, Yuan Zhang, Tillmann Klamroth and Luxia Wang\*

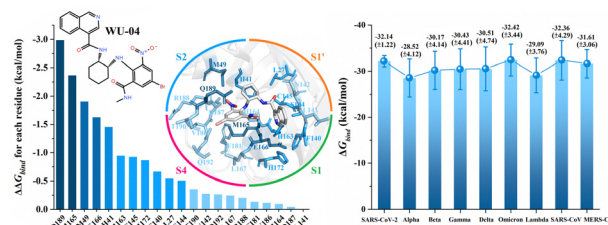


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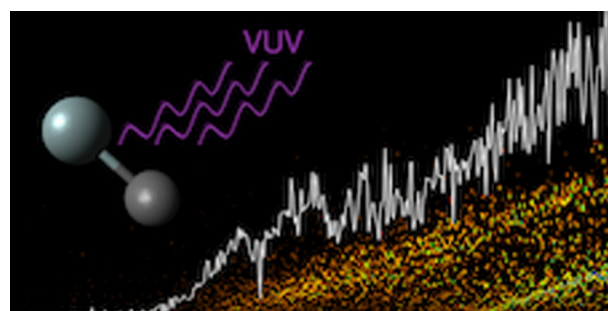
Jianhua Wu, Hong-Xing Zhang\* and Jilong Zhang\*



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# Single-photon ionization of SiC in the gas phase: experimental and *ab initio* characterization of $\text{SiC}^+$

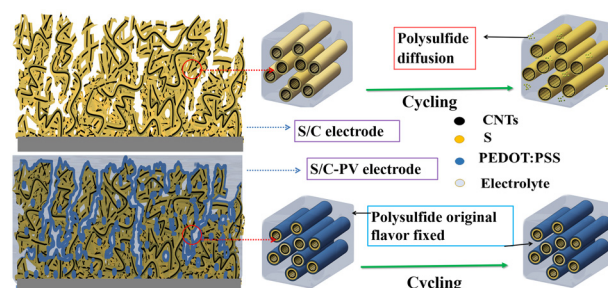
B. Gans,\* J. Liévin, P. Halvick, N. L. Chen, S. Boyé-Péronne, S. Hartweg, G. A. Garcia and J.-C. Loison



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# Enhanced cycling stability of Li–sulfur battery composites by low pressure penetration of PEDOT:PSS coating

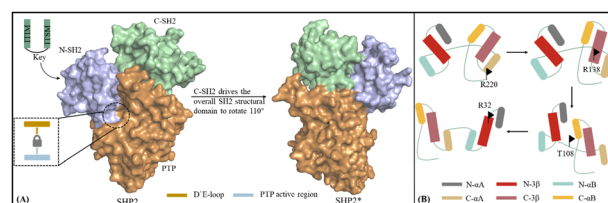
Qiang Huang, Guojun Zha,\* Zhaoyu Hu, Hangzhong Liu, Seema Agarwal and Haoqing Hou\*



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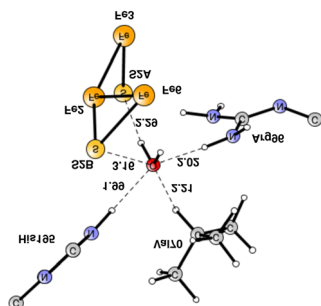
# Study on the allosteric activation mechanism of SHP2 via elastic network models and neural relational inference molecular dynamics simulation

Ling Liu, Yan Cheng, Zhigang Zhang, Jing Li, Yichao Geng, Qingsong Li, Daxian Luo, Li Liang, Wei Liu, Jianping Hu and Weiwei Ouyang\*



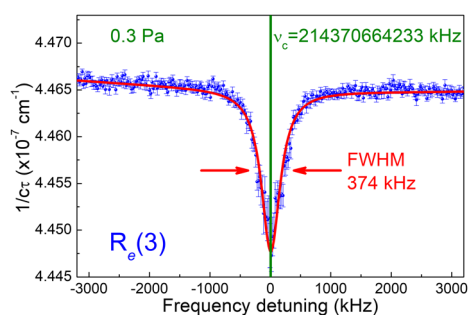
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The mechanism for N<sub>2</sub> activation in the E<sub>4</sub> – state of nitrogenase

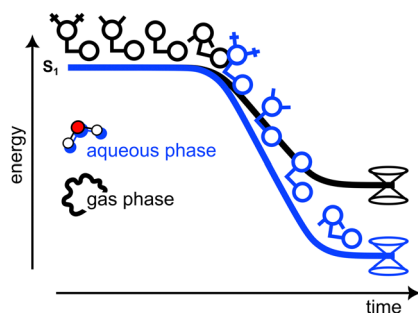
Per E. M. Siegbahn

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On the <sup>12</sup>C<sub>2</sub>H<sub>2</sub> near-infrared spectrum: absolute transition frequencies and an improved spectroscopic network at the kHz accuracy level

Antonio Castrillo, Eugenio Fasci, Tibor Furtenbacher, Vittorio D'Agostino, Muhammad A. Khan, Stefania Gravina, Livio Gianfrani\* and Attila G. Császár\*

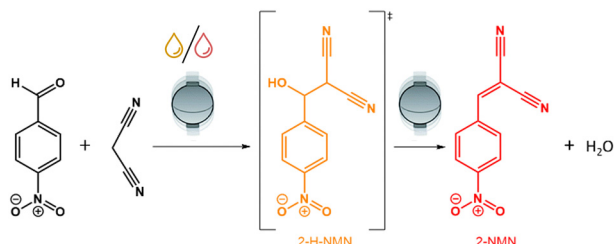
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## Alkylated green fluorescent protein chromophores: dynamics in the gas phase and in aqueous solution

Eleanor K. Ashworth, Min-Hsien Kao, Cate S. Anstöter, Gerard Riesco-Llach, Lluís Blancafort, Kyril M. Solntsev, Stephen R. Meech, Jan R. R. Verlet and James N. Bull\*

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Exploring the role of solvent polarity in mechanochemical Knoevenagel condensation: *in situ* investigation and isolation of reaction intermediates

Kerstin Scheurrell, Inês C. B. Martins,\* Claire Murray and Franziska Emmerling\*



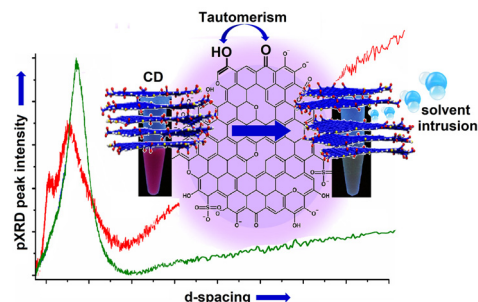


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# Elucidating the relationship between red fluorescence and structural dynamics of carbon dots dispersed in different solvents

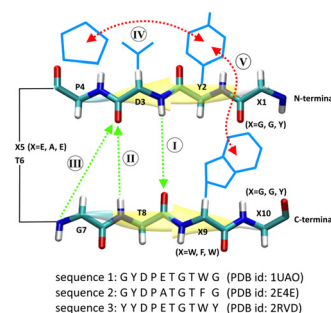
Saptarshi Mandal, Shakkira Erimban, Subhrajee Banerjee, Snehasis Daschakraborty\* and Prolay Das\*



23658

# A study of *ab initio* folding of chignolins using replica-exchange molecular dynamics simulations

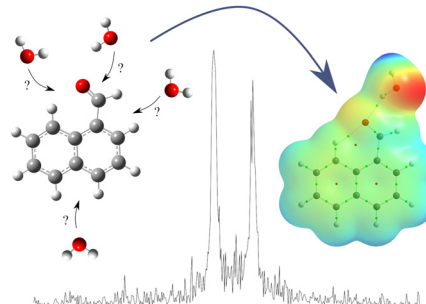
Guojie Cheng, Panpan Wang, Huihui Liu and Dawei Zhang\*



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# The hydration of an oxy-polycyclic aromatic compound: the case of naphthaldehyde

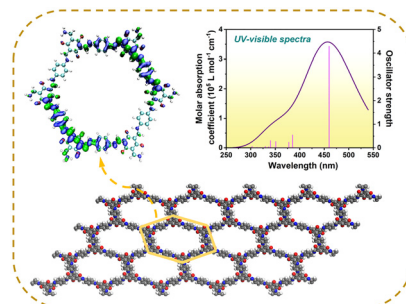
Jordan A. Claus, Celina Bermúdez, Valérie Vallet, Laurent Margulès and Manuel Goubet\*



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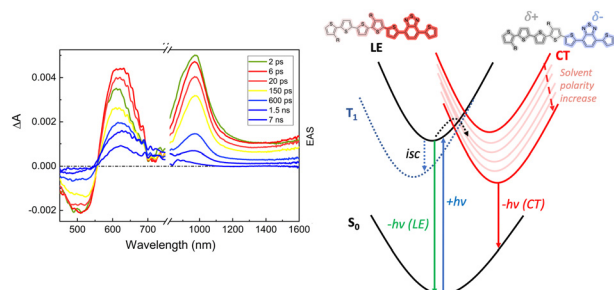
# Calculation of excited states of monolayer TPPA-COF based on first principles

Xudong Tang, Yani Liu, Mingyang Li, Wangyang Ding, Haihua Chen, Wenjuan Wei\* and Jiayu Li\*



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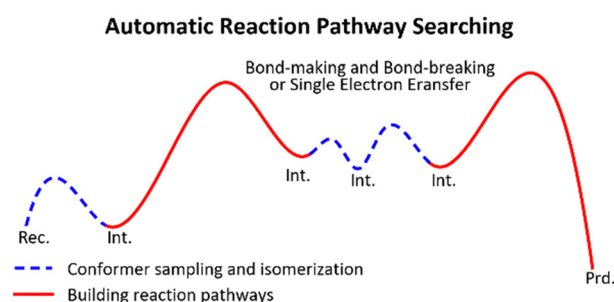
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### Photophysics and charge transfer in oligo(thiophene) based conjugated diblock oligomers

Habtom B. Gobeze, Pradeepkumar Jagadesan and Kirk S. Schanze\*

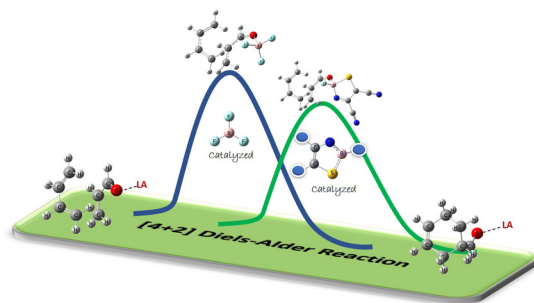
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### Combined molecular dynamics and coordinate driving method for automatically searching complicated reaction pathways

Guoao Li, Zhenxing Li, Liuzhou Gao, Shengda Chen, Guoqiang Wang\* and Shuhua Li\*

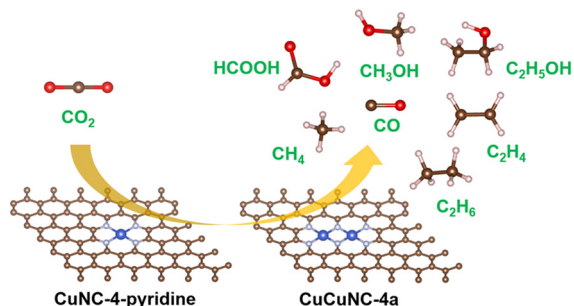
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### Insights into the catalytic activity of boron-doped thiazoles in the Diels–Alder reaction

Swapan Sinha, Abhishek Das and Santanab Giri\*

23717



### Theoretical exploration on the performance of single and dual-atom Cu catalysts on the CO<sub>2</sub> electroreduction process: a DFT study

Zhongze Bai, Xi Zhuo Jiang\* and Kai H. Luo\*

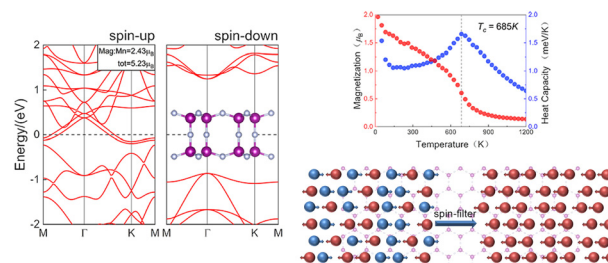


## RESEARCH PAPERS

23728

# Bilayer hexagonal structure $\text{MnN}_2$ nanosheets with room-temperature ferromagnetic half-metal behavior and a tunable electronic structure

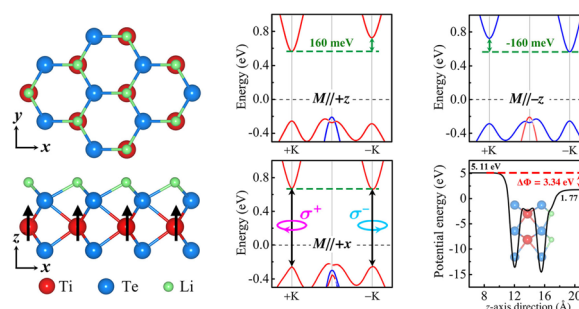
Yuan Gao, Honggang Pan\* and Baozeng Zhou\*



23738

# Piezoelectricity and valley polarization in a semilithiated $2\text{H-TiTe}_2$ monolayer with near room-temperature ferromagnetism

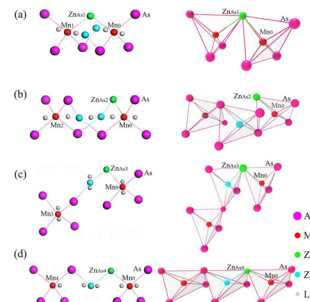
Kang Sheng, Bokai Zhang and Zhi-Yong Wang\*



23746

# Tuning the magnetic ordering driven by cationic antisite defects in the $\text{Li}(\text{ZnMn})\text{As}$ system

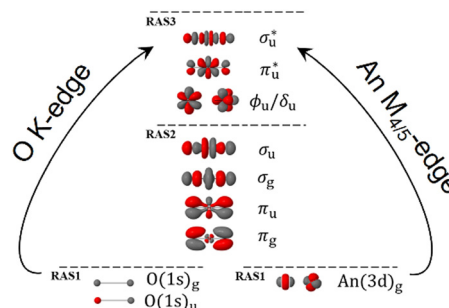
ManFu Wang, WeiJia Tang, JinGang Zhang, SiFan Wang, JingSheng Xu, HaoXu Wang, GuiBing Pang,\* ZhiHua Zhang\* and Zhong Lan



23753

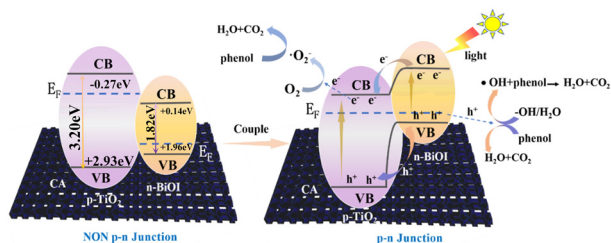
# Bounding $[\text{AnO}_2]^{2+}$ ( $\text{An} = \text{U}, \text{Np}$ ) covalency by simulated O K-edge and An M-edge X-ray absorption near-edge spectroscopy

Kurtis Stanistreet-Welsh and Andrew Kerridge\*



## RESEARCH PAPERS

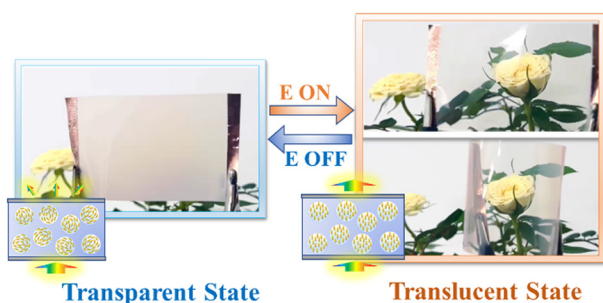
23761



### Preparation and performance of aerogel-based BiOI/TiO<sub>2</sub> heterojunction photoelectrocatalytic electrodes

Juanqin Xue, Peng Wang, Wen Cheng, Long Shi and Qiang Bi\*

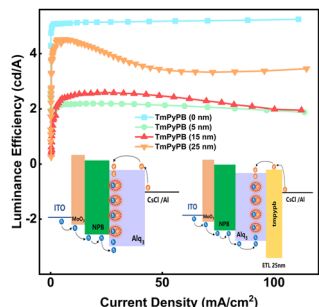
23770



### Balanced electro-optical properties and off-axis haze performance of a polymer-dispersed liquid crystal film via refractive index matching

Meina Yu,\* Jianjun Xu, Luoning Zhang, Qian Wang, Cheng Zou, Yanzi Gao\* and Huai Yang\*

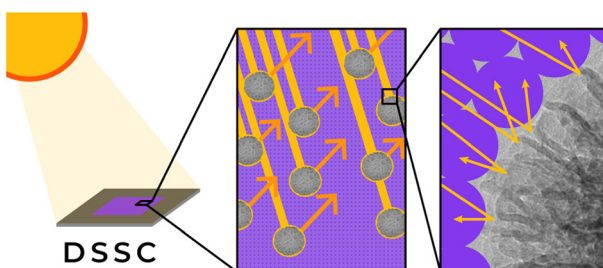
23783



### Investigations on exciton recombination and annihilation in TmPyPB-ETL OLEDs using magnetic field effects

Jiayi Song, Yunxia Guan,\* Cheng Wang, Xi Bao, Wanjiao Li, Lijia Chen and Lianbin Niu\*

23792



### A morphological study of bicontinuous concentric lamellar silica synthesized at atmospheric pressure and its application as an internal micro-reflector in dye-sensitized solar cells

Nadiatus Silmi, Rafiq Arsyad, Didi Prasetyo Benu, Fairuz Gianirfan Nugroho, Wiji Lestari Khasannah, Muhammad Iqbal, Brian Yuliarto, Rino Rakhmata Mukti and Veinardi Suendo\*



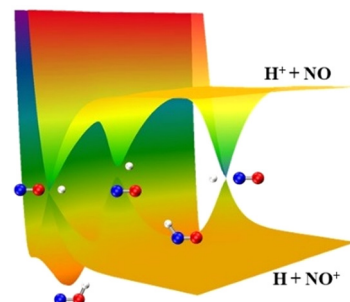


## RESEARCH PAPERS

23808

Nonadiabatic quantum dynamics of the charge transfer reaction  $\text{H}^+ + \text{NO}(X^2\Pi) \rightarrow \text{H} + \text{NO}^+(X^1\Sigma^+)$ 

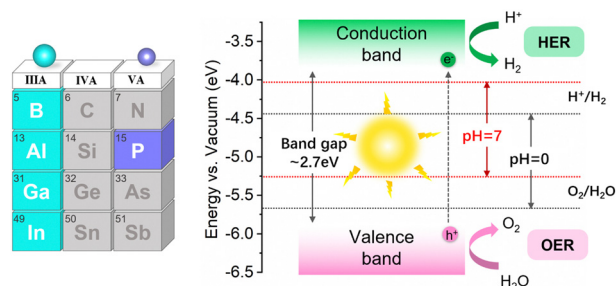
Zhimo Wang, Siting Hou and Changjian Xie\*



23819

Penta-MP<sub>5</sub> (M = B, Al, Ga, In) monolayers as high-performance photocatalysts for overall water splitting

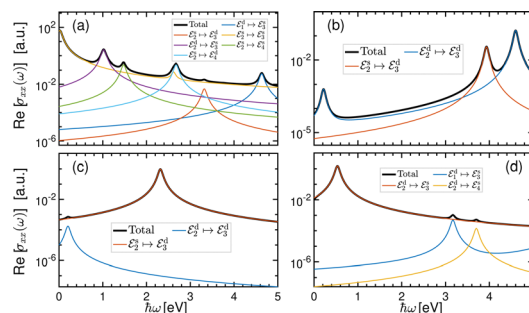
Jiao Chen, Xinyong Cai,\* Xiaotao Zhang, Hongyan Wang,\* Yuxiang Ni, Xuefei Liu and Yuanzheng Chen\*



23829

On the impact of adsorbed gas molecules on the anisotropic electro-optical properties of  $\beta_{12}$ -borophene

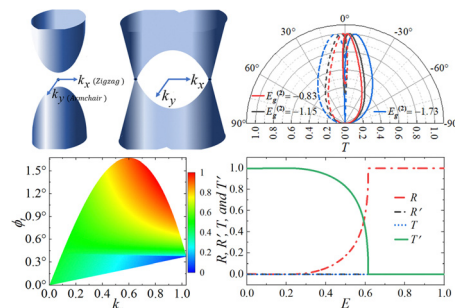
Nguyen N. Hieu, Chuong V. Nguyen, Huynh V. Phuc and Bui D. Hoi\*



23836

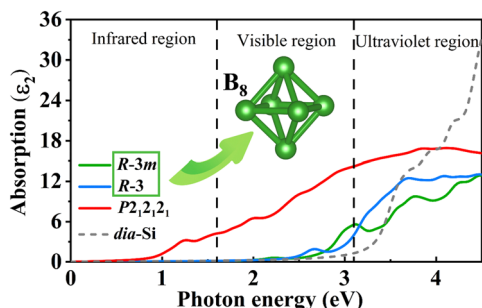
## Anomalous Klein tunneling in two-dimensional black phosphorus heterojunctions

Shu-Gang Chen, Bin-Yuan Zhang, Zi-Wei Yang and Wei-Jiang Gong\*



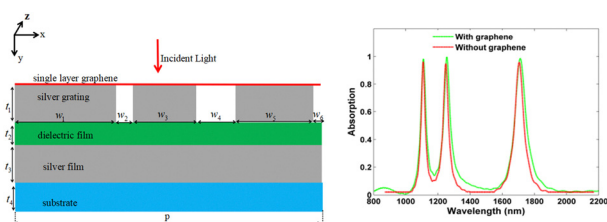
## RESEARCH PAPERS

23847

Exploration of  $AB_3Si_3$  ( $A = Na/K/Rb/Cs$ ) compounds under moderate pressure

Xiangyue Cui, Miao Zhang\* and Lili Gao\*

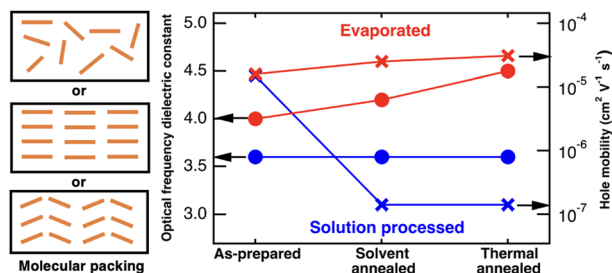
23855



## A TM polarization absorber based on a graphene–silver asymmetrical grating structure for near-infrared frequencies

Wenxing Wang, Yuchang Li, Fang Chen,\* Shubo Cheng, Wenxing Yang, Boyun Wang and Zao Yi

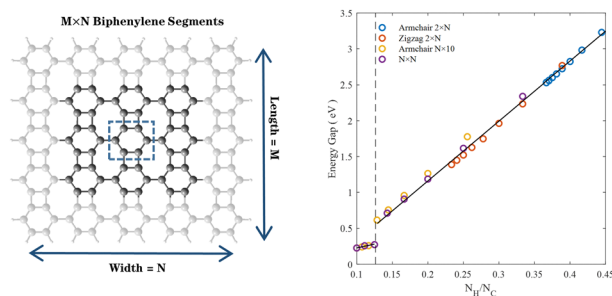
23867



## The impact of film deposition and annealing on the nanostructure and dielectric constant of organic semiconductor thin films

Lachlan Packman, Neil Mallo, Aaron Raynor, Mile Gao, Mohammad Babazadeh, Hui Jin, David M. Huang, Paul L. Burn,\* Ian R. Gentle\* and Paul E. Shaw

23879



## Size-tunable energy gaps of hydrogen-terminated biphenylene segments

Yirui Lu, Lei Yan,\* Huixia Fu,\* Yuhui Song, Yifei Cao, Sen Li, Ruhai Du, Jinping Li, Zhengkun Fu and Zhenglong Zhang\*

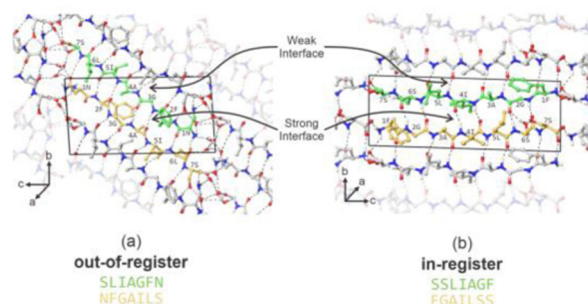


## RESEARCH PAPERS

23885

### Effect of strand register in the stability and reactivity of crystals from peptides forming amyloid fibrils

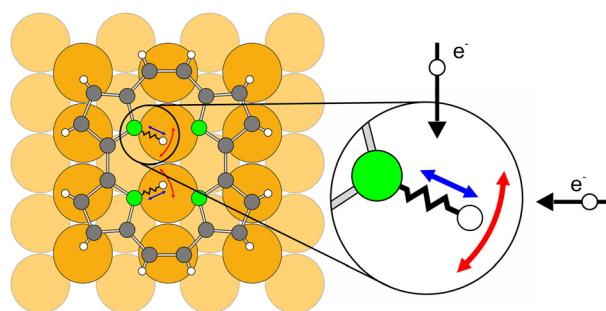
Camila Muñoz-Gutiérrez, Francisco Adasme-Carreño, Jans Alzate-Morales and Joel Ireta\*



23894

### Anisotropic coupling of individual vibrational modes to a Cu(110) substrate

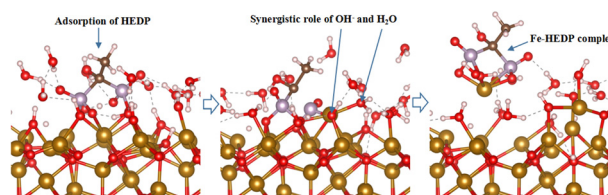
Andreas Christ,\* Patrick Härtl, Manuel Seitz, Tobias Edelmann, Matthias Bode, Jacek Waluk and Markus Leisegang



23901

### Dissolution mechanism of Fe<sub>3</sub>O<sub>4</sub> scale by 1-hydroxyethane-1,1-diphosphonic acid: an *ab initio* molecular metadynamics study

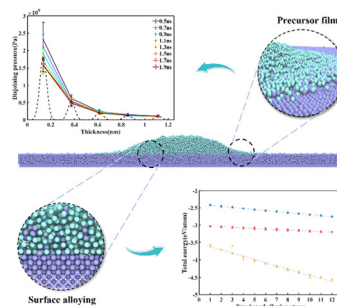
Xiaoyang Zhao, Guo Jin, Ding Guo, Xin Xiao, Junmin Nan\* and Chen Wu\*



23909

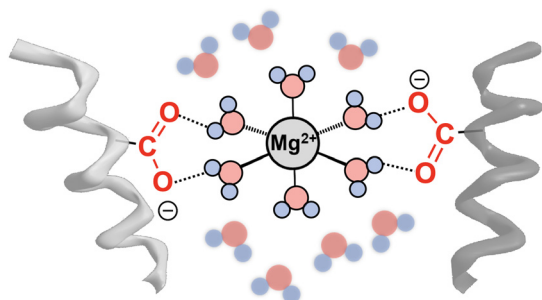
### The formation mechanism of the precursor film in high temperature molten metal systems: insight into structural disjoining pressure

Yuren Zhao, Masahiko Shibahara, Xingyu Fan, Wenhe Zhang, Chong Liu and Jingmin Li\*



## RESEARCH PAPERS

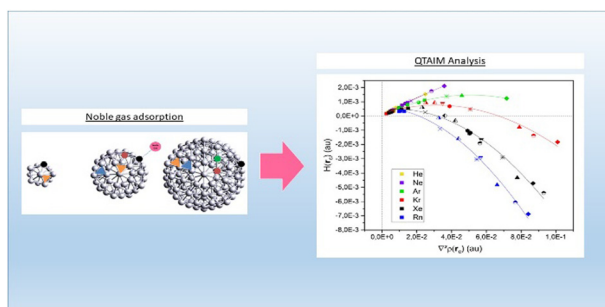
23923



### Stepwise hydration of $[\text{CH}_3\text{COOMg}]^+$ studied by cold ion trap infrared spectroscopy: insights into interactions in the magnesium channel selection filters

Hikaru Takayanagi, Jean-Xavier Bardaud, Keisuke Hirata, Valérie Brenner, Eric Gloaguen,\* Shun-ichi Ishiuchi\* and Masaaki Fujii\*

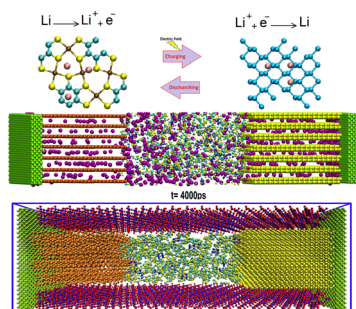
23929



### On the nature of noble gas – metal bond in silver aggregates

Celian Courtney and Bruno Siberchicot\*

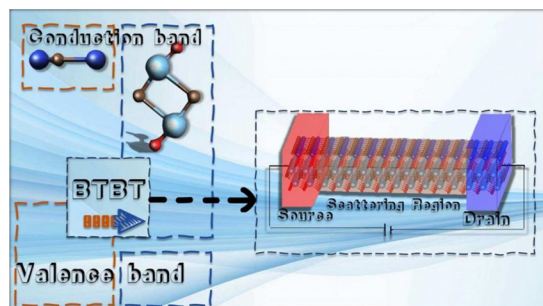
23937



### Toward efficient electrodes for a high-performance fast-charge Li-ion battery: molecular dynamics simulation and DFT calculations

Ameneh Zaboli, Heidar Raissi,\* Hassan Hashemzadeh and Farzaneh Farzad

23954



### A novel broken-gap chemical-bonded SiC/Ti<sub>2</sub>CO<sub>2</sub> heterojunction with band to band tunneling: first-principles investigation

Zhuo-Ni Dai, Wei Sheng, Xiao-Ying Zhou, Jie Zhan and Ying Xu\*



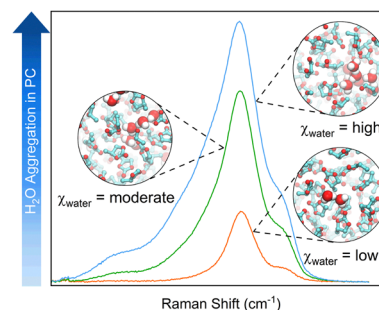


## RESEARCH PAPERS

23963

# Structural evolution of water-in-propylene carbonate mixtures revealed by polarized Raman spectroscopy and molecular dynamics

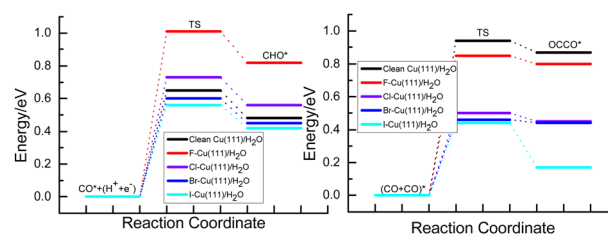
Jessica B. Clark, Tai Bowling-Charles, Shamma Jabeen Proma, Biswajit Biswas, David T. Limmer and Heather C. Allen\*



23977

# Theoretical understanding of the effect of specifically adsorbed halide anions on Cu-catalyzed CO<sub>2</sub> electroreduction activity and product selectivity

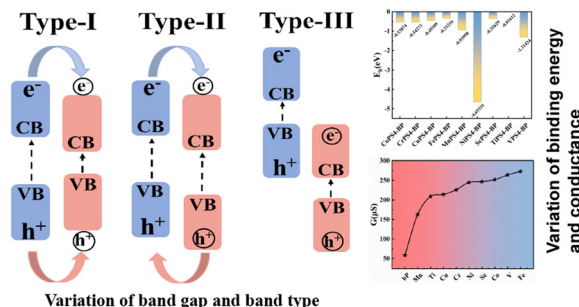
Lihui Ou,\* Wanli You,\* Junling Jin and Yuandao Chen



23988

# Interface engineering strategy for multisource spintronic devices via TMPS<sub>4</sub> modulation of black-phosphorus

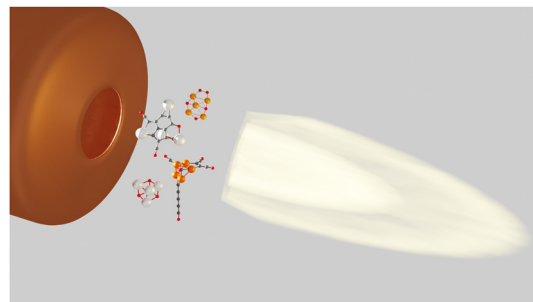
Tongtong Wang, Fangqi Liu, Sheng Liu, Bin Liu and Sicong Zhu\*



23995

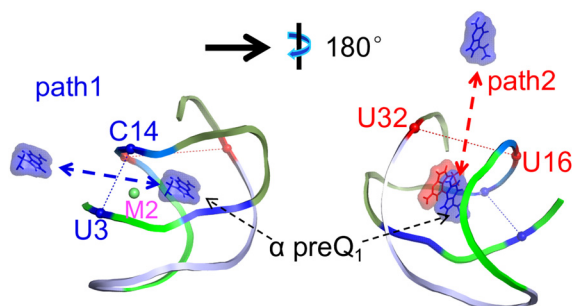
# Accounting for super-, plateau- and mesa-rate burning by lead and copper-based ballistic modifiers in double-base propellants: a computational study

Lisette R. Warren, Aaron Rowell, Patrick McMaster, Colin R. Pulham and Carole A. Morrison\*



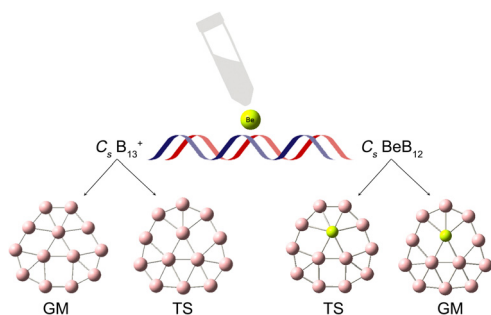
## RESEARCH PAPERS

24004

**Dynamical characterization and multiple unbinding paths of two PreQ<sub>1</sub> ligands in one pocket**

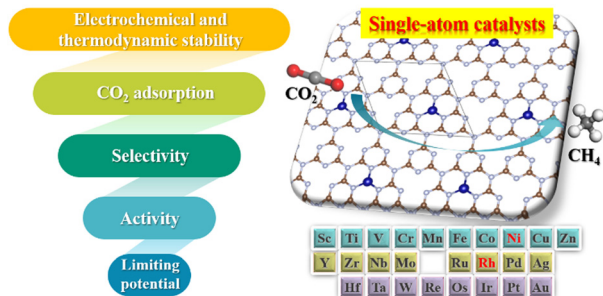
Guodong Hu,\* Yonghong Zhang, Zhiping Yu, Tiejun Cui and Wanling Cui

24016

**Isovalent electronic systems B<sub>13</sub><sup>+</sup> and BeB<sub>12</sub>: structural interchange of GM and TS**

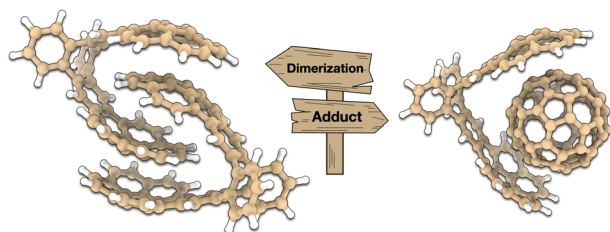
Ceng Zhang, Hai-Ru Li,\* Rui-Hua Zhou, Yan Zhang and Xiong-Bo Duan\*

24022

**Computational screening of high activity and selectivity of CO<sub>2</sub> reduction via transition metal single-atom catalysts on triazine-based graphite carbon nitride**

Shuang Ji, Yi Li,\* Yongfan Zhang and Wei Lin\*

24031

**When catchers meet – a computational study on the dimerization of the Buckycatcher**

Filipe Menezes\* and Grzegorz Maria Popowicz\*

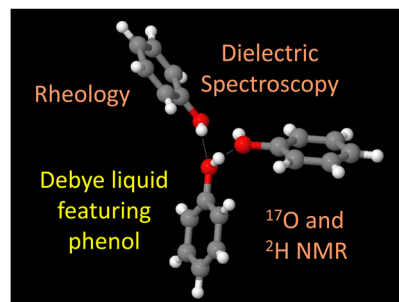


## RESEARCH PAPERS

24042

# Phenol, the simplest aromatic monohydroxy alcohol, displays a faint Debye-like process when mixed with a nonassociating liquid

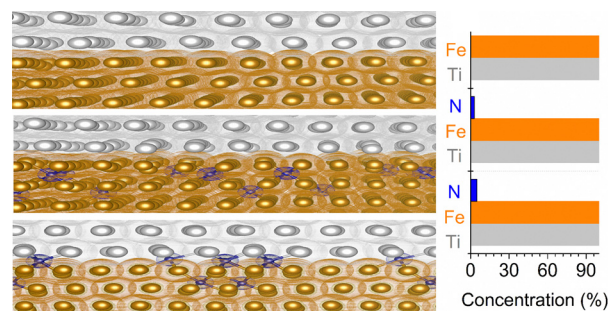
Lars Hoffmann, Joachim Beerwerth, Kevin Moch and Roland Böhmer



24060

# The nitriding effect on the stability and mechanical properties of the iron titan phase: first-principles investigation

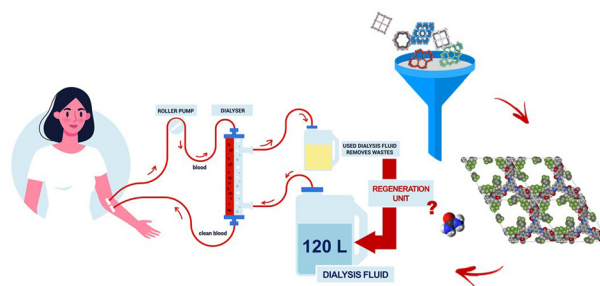
Andrey D. Ishkildin, Andrey A. Kistanov,\*  
Artem A. Izosimov and Elena A. Korznikova



24069

# *In silico* screening of nanoporous materials for urea removal in hemodialysis applications

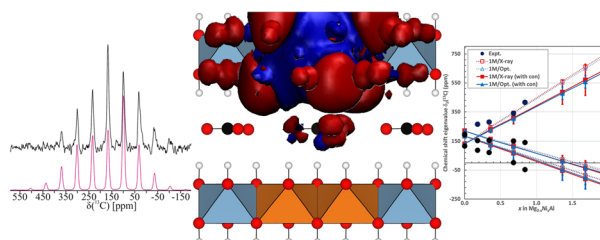
Thomas Fabiani, Eleonora Ricci, Cristiana Boi,  
Simone Dimartino and Maria Grazia De Angelis\*



24081

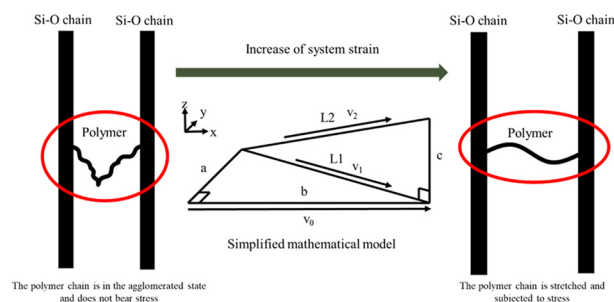
# Unravelling the effect of paramagnetic Ni<sup>2+</sup> on the <sup>13</sup>C NMR shift tensor for carbonate in Mg<sub>2-x</sub>Ni<sub>x</sub>Al layered double hydroxides by quantum-chemical computations

Megha Mohan, Anders B. A. Andersen, Jiří Mareš,  
Nicolai Dugaard Jensen, Ulla Gro Nielsen\* and Juha Vaara\*



## RESEARCH PAPERS

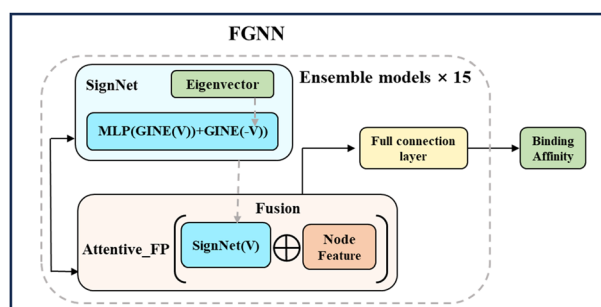
24097



### A toughening mechanism of the strain rate-optimal chain length on polymer-modified calcium silicate hydrates (CSH)

Yang Zhou,\* Shuai Xiao, Luqing Cheng, Yuan Chen, JinHui Tang and Wei She

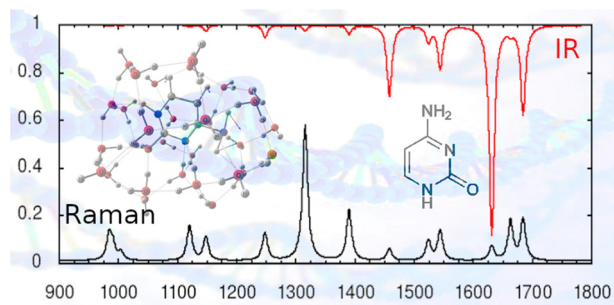
24110



### Ligand binding affinity prediction with fusion of graph neural networks and 3D structure-based complex graph

Lina Dong, Shuai Shi, Xiaoyang Qu, Ding Luo and Binju Wang\*

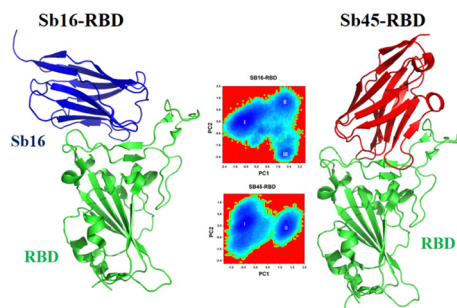
24121



### Computational analysis of the vibrational spectra and structure of aqueous cytosine

Sergey A. Katsyuba\* and Timur I. Burganov

24129



### Binding of synthetic nanobodies to the SARS-CoV-2 receptor-binding domain: the importance of salt bridges

Hujun Shen\* and Hengxiu Yang

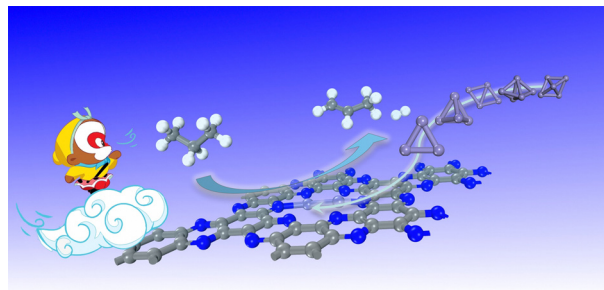


## RESEARCH PAPERS

24143

### Mechanism research reveals the role of $\text{Fe}_n$ ( $n = 2-5$ ) supported $\text{C}_2\text{N}$ as single-cluster catalysts (SCCs) for the non-oxidative propane dehydrogenation in the optimization of catalytic performance

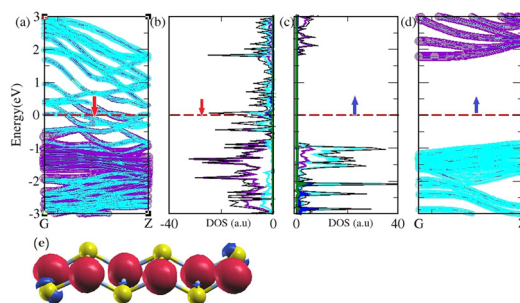
Yu Zhang, Qin Chen and Hui Zhang\*



24155

### Ferromagnetic half-metal with high Curie temperature in Cr P nanoribbons: good material for spintronic applications

Tayebeh Movlaroooy\* and Adeleh Vatankhahan



## CORRECTIONS

24163

### Correction: Increasing ion yield circular dichroism in femtosecond photoionisation using optimal control theory

Manel Mondelo-Martell, Leon A. Kerber, Daniel Basilewitsch, Hendrike Braun, Christiane P. Koch and Daniel M. Reich\*

24168

### Correction: A label-free aptamer-based nanogap capacitive biosensor with greatly diminished electrode polarization effects

Zahra Saribal

