

## IN THIS ISSUE

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### Cover

See Y. Stergiou, K. Schwarzenberger *et al.*, pp. 2920–2926. Image reproduced by permission of Y. Stergiou from *Phys. Chem. Chem. Phys.*, 2025, 27, 2920.



### Inside cover

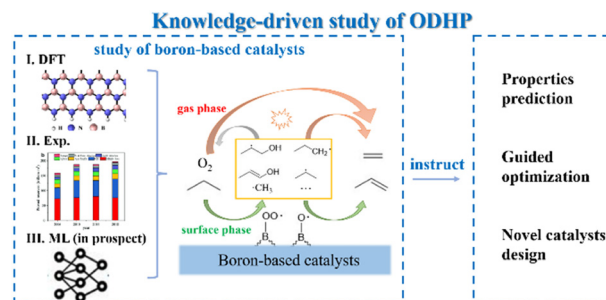
See Daniel Jezierski, José Lorenzana and Wojciech Grochala, pp. 2927–2938. Image reproduced by permission of Daniel Jezierski from *Phys. Chem. Chem. Phys.*, 2025, 27, 2927.

## PERSPECTIVE

2874

### Knowledge-driven design of boron-based catalysts for oxidative dehydrogenation of propane

Weixi Chen, Ziyi Liu, Lihan Zhu and Dongqi Wang\*

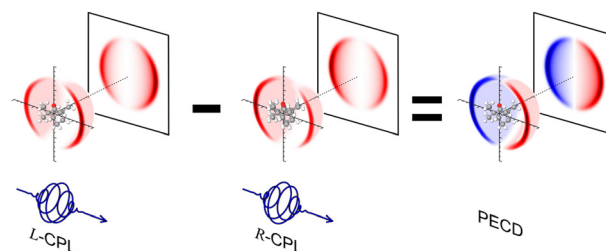


## TUTORIAL REVIEW

2888

### Two decades of imaging photoelectron circular dichroism: from first principles to future perspectives

Chris Sparling and Dave Townsend\*



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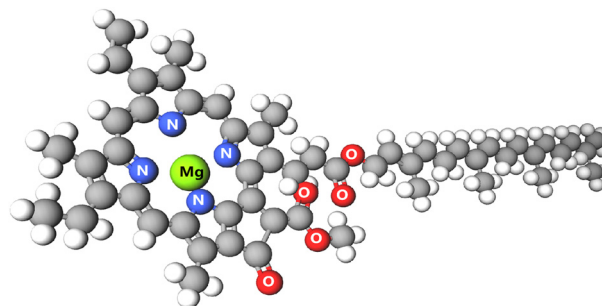
Fundamental questions  
Elemental answers

## REVIEW

2908

**Theory for ultrafast energy transfer in photosynthesis**

Jingyu Liu, Tao-Yuan Du,\* Xuan Deng, Bo Li, Qianqian Cheng, Jiangong Hu and Kaiyao Huang

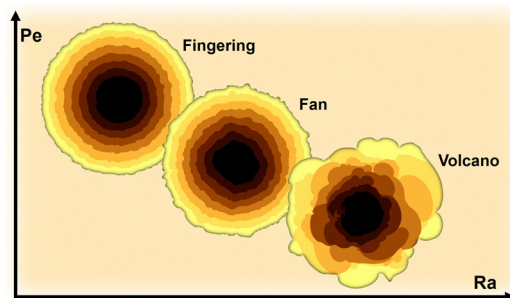


## RESEARCH PAPERS

2920

**Flow-driven pattern formation during coacervation of xanthan gum with a cationic surfactant**

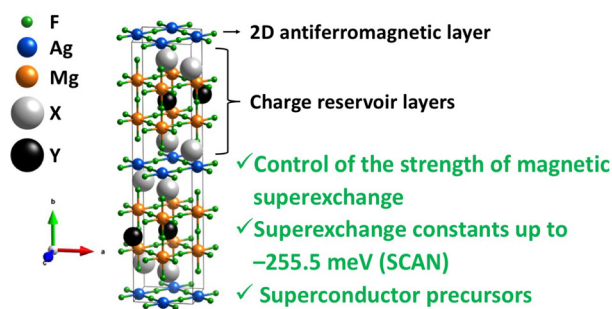
Y. Stergiou,\* A. Perrakis, A. De Wit and K. Schwarzenberger\*



2927

**Controlling orbital ordering of intergrowth structures with flat  $[\text{Ag}^{\text{II}}\text{F}_2]$  layers to mimic oxocuprates(II)**

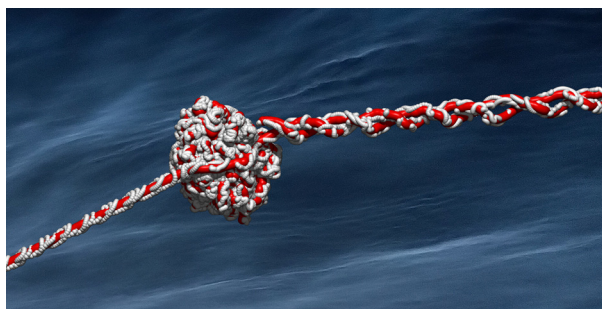
Daniel Jezierski,\* José Lorenzana\* and Wojciech Grochala\*



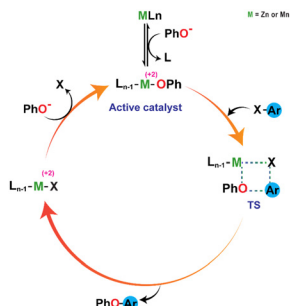
2939

**Molecular dynamics of evaporative cooling of water clusters**

Martin Klíma, Jiří Janek and Jiří Kolafa\*



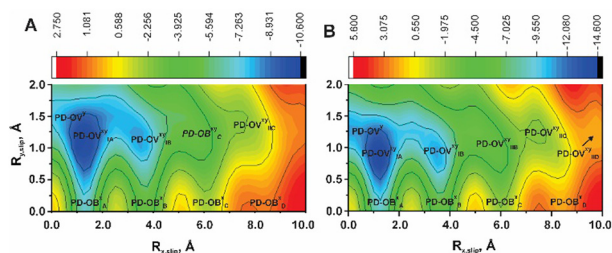
2948



### Unveiling the molecular mechanism of Mn and Zn-catalyzed Ullmann-type C–O cross-coupling reactions

C. Rajalakshmi, Parvathi Santhoshkumar, Lydia Elizabeth Mathews, Ann Miriam Abraham, K. R. Rohit, Gopinathan Anilkumar and Vibin Ipe Thomas\*

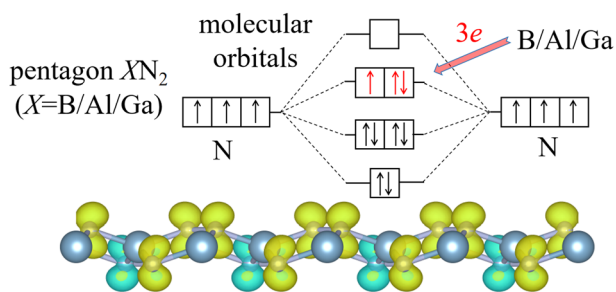
2958



### Stack bonding in pentacene and its derivatives

Craig A. Bayse

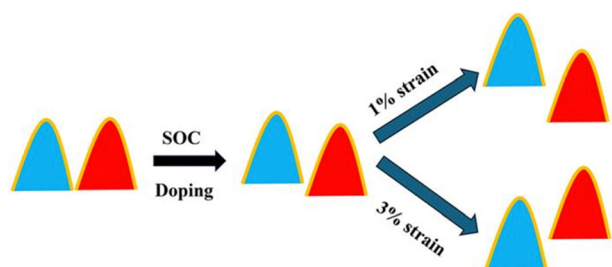
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### High Néel temperature and magnetism modulation in 2D pentagon-based $XN_2$ ( $X = B, Al, \text{ and } Ga$ ) structures with spin-polarized non-metallic atoms

Zhenyu Wu and Hong Zhang\*

2977



### Enhancing valley splitting and anomalous valley Hall effect in the V-doped Janus MoSeTe monolayer

Shulai Lei, Jiayao Wang, Rongli Zhao,\* Jinbo Sun, Shujuan Li,\* Xinyue Xiong, Yin Wang and Ke Xu\*

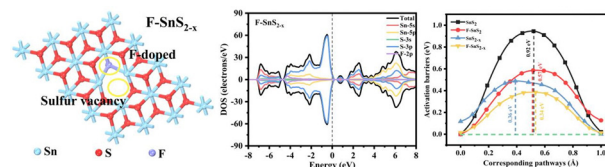


## RESEARCH PAPERS

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### The effect of introducing fluorine doping and sulfur vacancies on SnS<sub>2</sub> as the anode electrode of LIBs: a density functional theory study

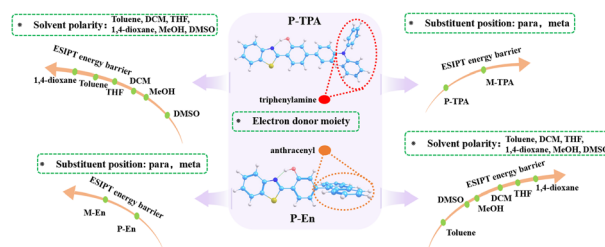
Jiayi Guan, Kaihui Lin, Yanbing Liao, Zhiling Xu, Yuda Lin\* and Shenghui Zheng\*



2993

### Elaborating H-bonding effect and excited state intramolecular proton transfer of 2-(2-hydroxyphenyl)benzothiazole based D- $\pi$ -A fluorescent dye

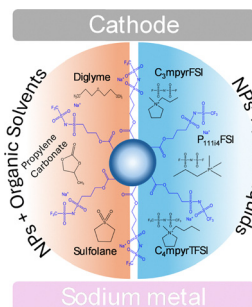
Xiu-Min Liu, Yin Yu, Shu-Ying Xu and Xue-Hai Ju\*



3006

### Gel polymer electrolytes based on sulfonamide functional polymer nanoparticles for sodium metal batteries

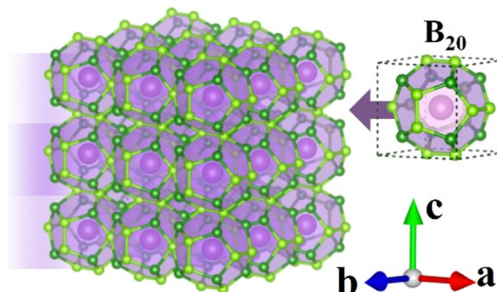
Pierre L. Stigliano,\* Antonela Gallastegui, Thomas H. Smith, Luke O'Dell, David Mecerreyes, Cristina Pozo-Gonzalo and Maria Forsyth\*



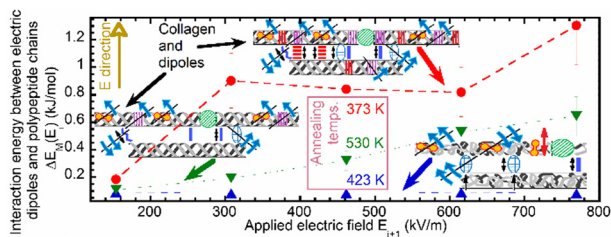
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### Superconductivity and high hardness in scandium-borides under pressure

Xiangru Tao, Aiqin Yang, Yundi Quan\* and Peng Zhang\*



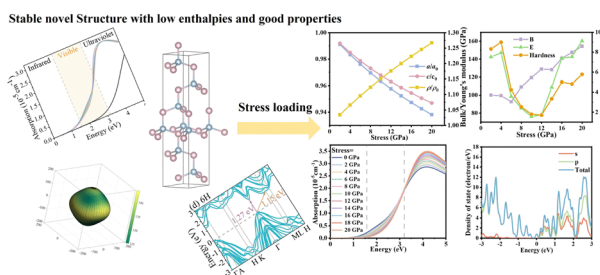
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### The mobility of polypeptide chains in cow femur bones controlled by an electric field

Fernando Daniel Lambri, Federico Guillermo Bonifacich, Melania Lucila Lambri, Mariel Antonella Lambri, Ricardo Raúl Mocellini, Griselda Irene Zelada and Osvaldo Agustin Lambri\*

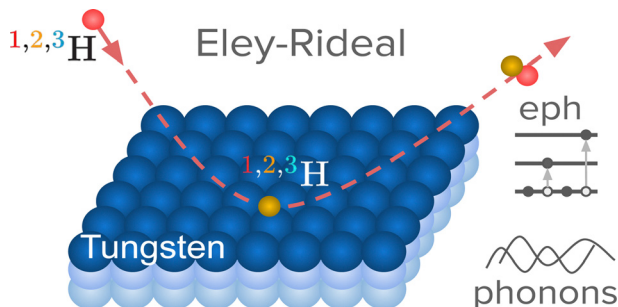
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### A dozen predicted SiGe alloys with low enthalpies and strong absorption of sunlight for photovoltaic applications

Zehao Lin, Qingyang Fan, Qing Pang, Jin Zhong Zhang, Dangli Gao\* and Yuling Song

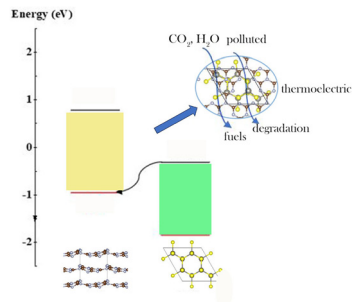
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### Isotope effects in Eley-Rideal abstraction of hydrogen from tungsten surfaces: the role of dissipation

Oihana Galparsoro,\* Raidel Martin-Barrios,\* Paulo Enrique Ibañez-Almaguer, Maykel Márquez-Mijares, José David Cremé, Yosvany Silva-Solis, Jesús Rubayo-Soneira, Cédric Crespos and Pascal Larregaray

3061



### The theoretical investigation of the g-C<sub>3</sub>N<sub>4</sub>/ZnS heterojunction for photocatalytic applications

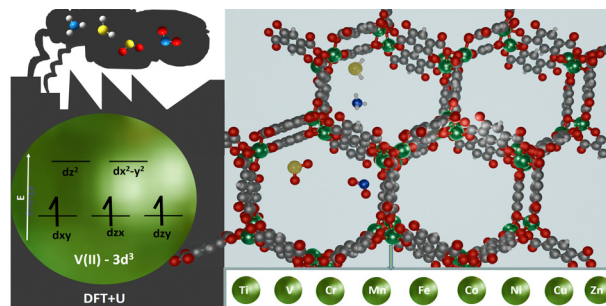
Elnaz Ranjbakhsh and Mohammad Izadyar\*



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### Comprehensive DFT investigation of small-molecule adsorption on the paradigm M-MOF-74 family of metal–organic frameworks

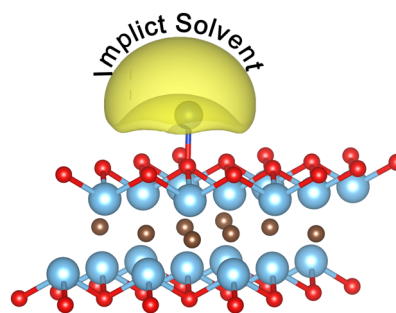
Nazli Jodaeasl, Shiliang Wang, Anguang Hu and Gilles H. Peslherbe\*



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### Single-atom lead ion adsorption behavior on $\text{Ti}_2\text{CO}_2$ MXene under different electrode potentials

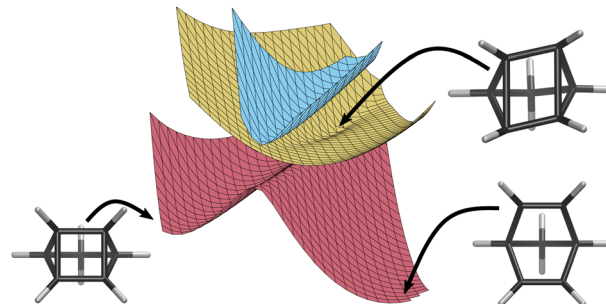
Kechen Li, Yang Ou, Yongzhi Wang, Jianbo Zhang and Yang Zhou\*



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### Electronic structure of norbornadiene and quadricyclane

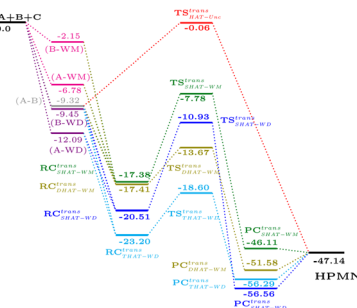
Joseph C. Cooper and Adam Kirrander\*



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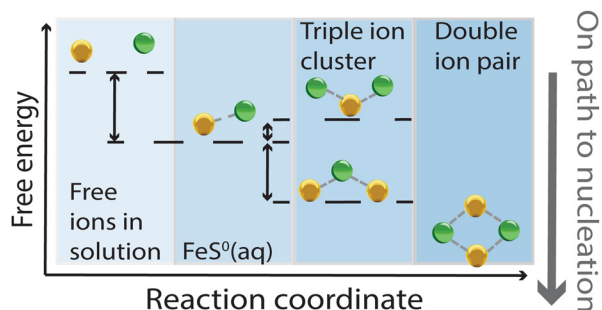
### Water as a catalyst in the reaction of nitrous acid (HONO) and Criegee intermediate ( $\text{CH}_2\text{OO}$ )

Vishva Jeet Anand, Vivek Kumar, Amit Kumar and Pradeep Kumar\*



## RESEARCH PAPERS

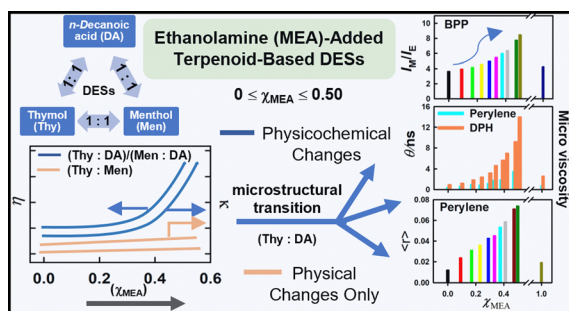
3115



### Influence of solution stoichiometry on the thermodynamic stability of prenucleation FeS clusters

Vincent F. D. Peters, Janou A. Koskamp, Devis Di Tommaso and Mariette Wolthers\*

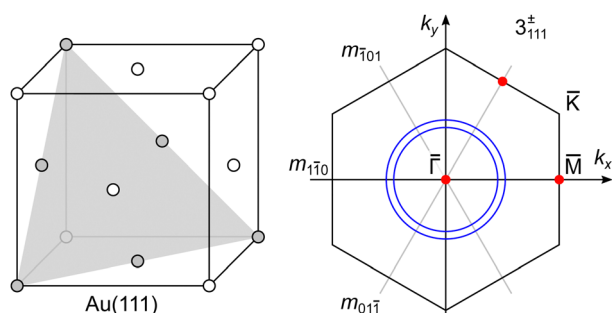
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### Ethanolamine-mediated microstructural transitions within terpenoid- and fatty acid-based deep eutectic solvents

Anjali and Siddharth Pandey\*

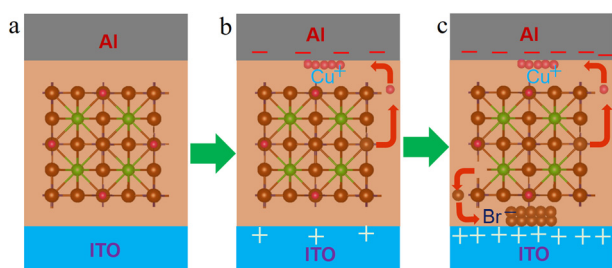
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### Rashba effect originates from the reduction of point-group symmetries

Koshi Okamura

3150



### Air-stable double halide perovskite $\text{Cs}_2\text{CuBiBr}_6$ : synthesis and memristor application

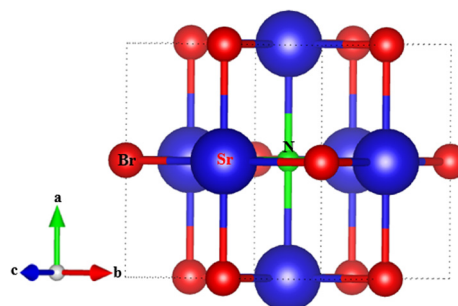
Atanu Betal, Anupam Chetia, Dibyajyoti Saikia, Krishnendu Karmakar, Ganesh Bera, Neha V. Dambhare, Arup K. Rath and Satyajit Sahu\*



3160

### Strain-dependent structural, electronic, mechanical, optical and thermoelectric properties of $\text{Sr}_3\text{NBr}_3$ perovskites for solar cell applications

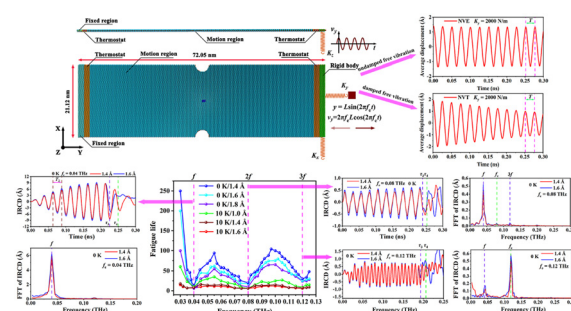
Amina, Naseem Akhter, Salhah Hamed Alrefaee, Anvar Nurmammedov, Mukhlisa Soliyeva, Pervaiz Ahmad, Vineet Tirth, Ali Algahtani, Q. Mohsen, O. Alsaqer, N. M. A. Hadia and Abid Zaman\*



3171

### Phononic origin of resonance in atomic scale fatigue of $\text{MoS}_2$

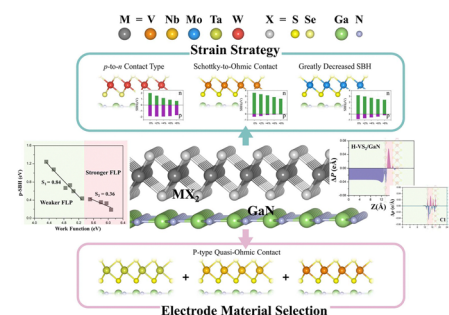
Yun Dong,\* Bo Shi, Yi Tao, Xinyi Tang, Jinguang Wang, Futian Yang and Yifan Liu



3185

### 2D metallic transition metal dichalcogenides: promising contact metals for 2D GaN-based (opto)electronic devices

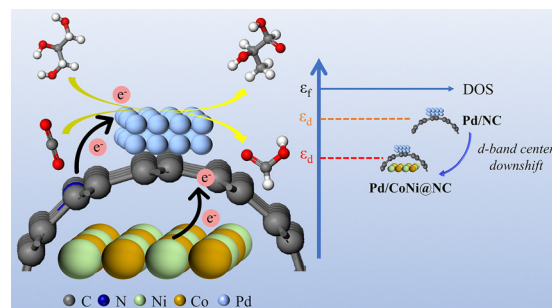
Jing Li, Lei Ao\* and Zhihua Xiong\*



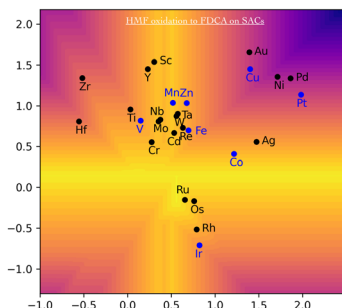
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### Tuning metal-support interactions in MOF-derived $\text{CoNi@NC}$ supported Pd catalysts for efficient hydrogenation of bicarbonate using glycerol as a hydrogen donor

Xiaojin Dong, Wenfeng Zhong, Xuecheng Li, Gang Wang, Hua Tan\* and Xinping Ouyang\*



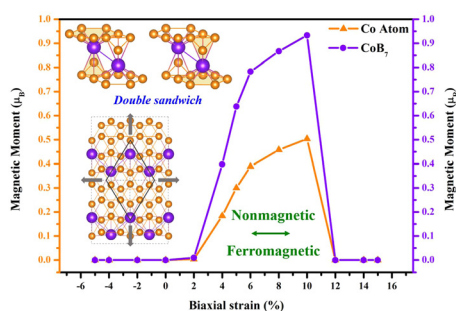
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### Nitrogen-doped graphene supported single-atom catalysts for efficient electrocatalytic oxidation of 5-hydroxymethylfurfural to 2,5-furandicarboxylic acid: a density functional theory study

Mingrong Li, Yungan Huang, Qiong Luo and Yongfei Ji\*

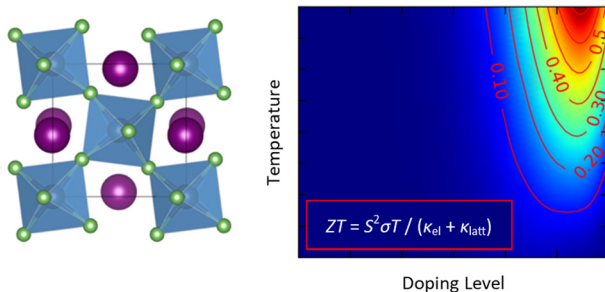
3217



### Two-dimensional inverse double sandwich CoB<sub>7</sub>: strain-induced non-magnetic to ferromagnetic transition

Liang Gu, Hui-Min Yang and Li-Ming Yang\*

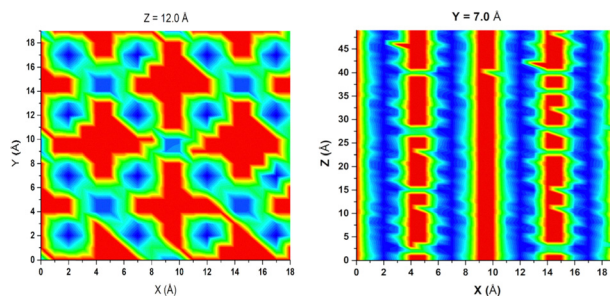
3230



### Thermoelectric properties of the low-spin lanthanide cobaltate perovskites LaCoO<sub>3</sub>, PrCoO<sub>3</sub>, and NdCoO<sub>3</sub> from first-principles calculations

Alveena Z. Khan, Joseph M. Flitcroft and Jonathan M. Skelton\*

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### Revisiting the in-plane and in-channel diffusion of lithium ions in a solid-state electrolyte at room temperature through neural network-assisted molecular dynamics simulations

Yao Huang, Dan Zhao, Mingsen Deng\* and Hujun Shen\*

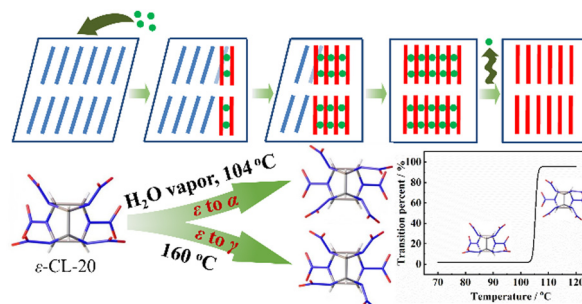


## RESEARCH PAPERS

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### Mechanism investigation on the solid–solid phase transition of CL-20 induced by water vapor

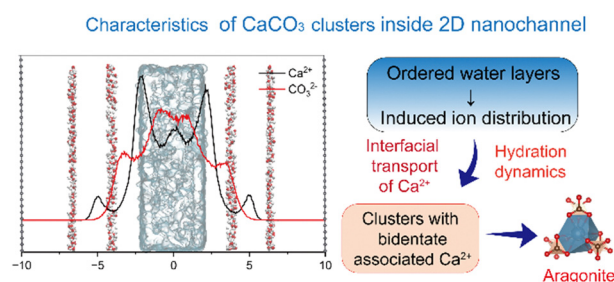
Ya Guo,\* Xueting Cai, Fangbao Jiao, Zhicheng Guo, Qi Huang and Qi Zhang\*



3263

### Microscopic insights into the effects of interfacial dynamics and nanoconfinement on characteristics of calcium carbonate clusters within two-dimensional nanochannels

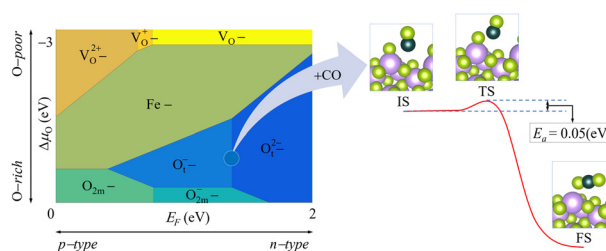
Jia-Ying Li, Rui-Tian Ma, Shi-Qi Zheng, Tian Xia and Hai-Bo Yi\*



3278

### Revealing the catalytic oxidation mechanism of CO on $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> surfaces: an *ab initio* thermodynamic study

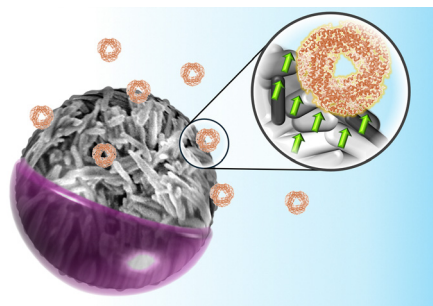
Yun-Hyok Song, Yun-Hyok Kye,\* Myong-Il Pang, Yong-Min Ho, Hyon-Chol Choe, Chol-Jun Yu\* and Chol-Yong Ri



3291

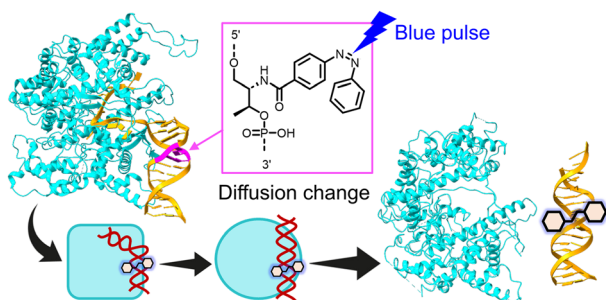
### Probing spin effects in phycocyanin using Janus-like ferromagnetic microparticles

Avi Schneider, Ilay David, Naama Goren, Hanna T. Fridman, Guy Lutzky, Shira Yochelis, Hagit Zer, Noam Adir, Nir Keren and Yossi Paltiel\*



## RESEARCH PAPERS

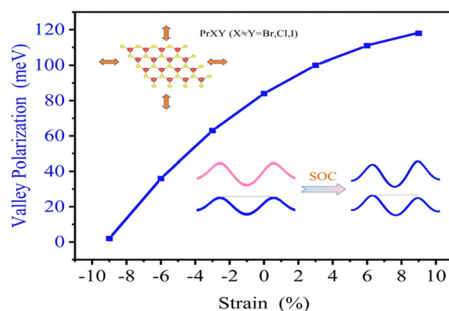
3302



### Reaction and interaction dynamics of azobenzene-tethered DNA with T7 RNA polymerase

Gennosuke Takekawa, Yusuke Nakasone, Yukiko Kamiya, Hiroyuki Asanuma and Masahide Terazima\*

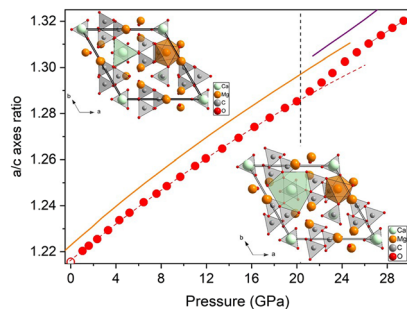
3313



### First-principles prediction of intrinsic ferrovalley properties in Janus rare-earth PrXY ( $X \neq Y = \text{Cl, Br, I}$ ) monolayers

Huai-Jin Zhang, Yuping Tian, Cui Jiang, Xiangru Kong\* and Wei-Jiang Gong\*

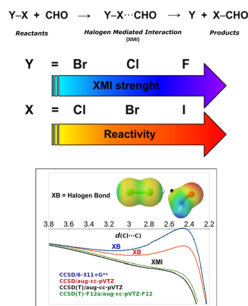
3320



### Pressure-driven phase transformations on $\text{Mg}_3\text{Ca}(\text{CO}_3)_4$ huntite carbonate

David Santamaría-Pérez,\* Raquel Chuliá-Jordán, Benedito Donizeti Botan-Neto, Ganesh Bera, Julio Pellicer-Porres, Lkhamsuren Bayarjargal, Alberto Otero-de-la-Roza and Catalin Popescu

3330



### The influence of halogen-mediated interactions on halogen abstraction reactions by formyl radicals

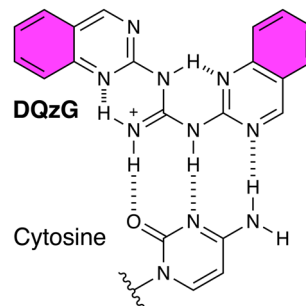
Matias O. Miranda, Darío J. R. Duarte\* and Victor M. Rayón\*



3341

### The role of spatial arrangement of aromatic rings on the binding of *N,N'*-diheteroaryl guanidine ligands to the G2C4/G2C4 motif DNA

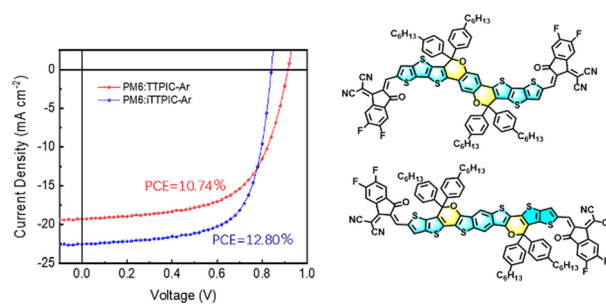
Eitaro Murakami, Tomonori Shibata,\* Megumi Tomemori, Gota Kawai and Kazuhiko Nakatani\*



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### Nonfullerene acceptors with carbon–oxygen-bridged fused nonacyclic donor units enable efficient organic solar cells

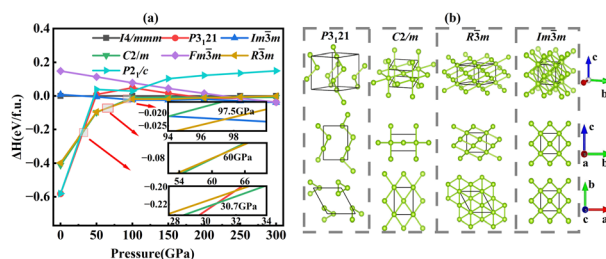
Jiamo Zhou, Xinying Ruan, Yufan Zhu, Ziqi Han, Jingyao Kong, Dan He\* and Fuwen Zhao\*



3357

### Phase transition and superconductivity of selenium under pressure

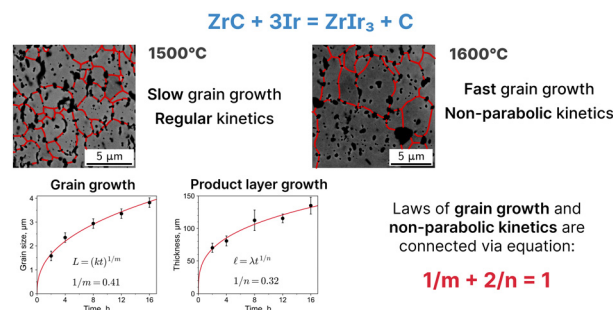
Enci Zuo, Yingying Chen,\* Gang Jiang, Liang Zhao and Jiguang Du\*



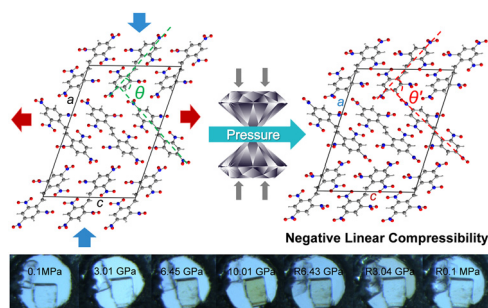
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### How grain structure evolution affects the kinetics of a solid-state reaction: a case of interaction between iridium and zirconium carbide

Yaroslav A. Nikiforov,\* Victoria A. Danilovsky and Natalya I. Baklanova



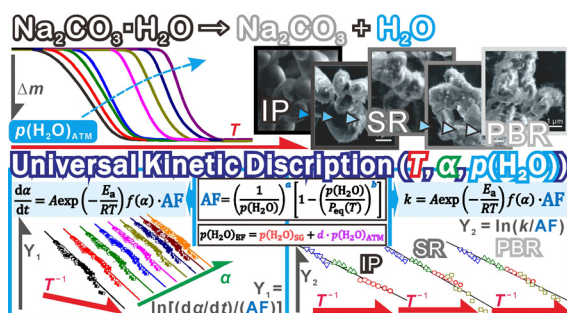
3375



### Negative linear compressibility and structural stability of the energetic material *trans*-hexanitrostilbene under pressure

Xinglong Deng, Dong Li, Boyang Fu, Yu Liu, Weilong He, Shourui Li\* and Weizhao Cai\*

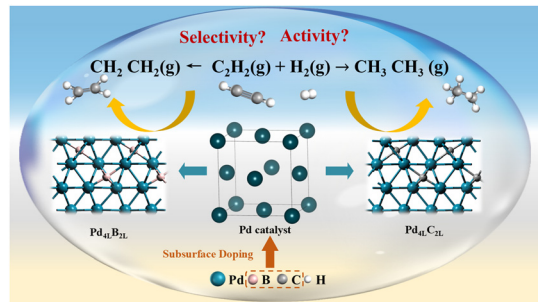
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### Universal kinetic description for the thermal dehydration of sodium carbonate monohydrate powder across different temperatures and water vapor pressures

Shunsuke Fukunaga, Yuto Zushi, Mito Hotta and Nobuyoshi Koga\*

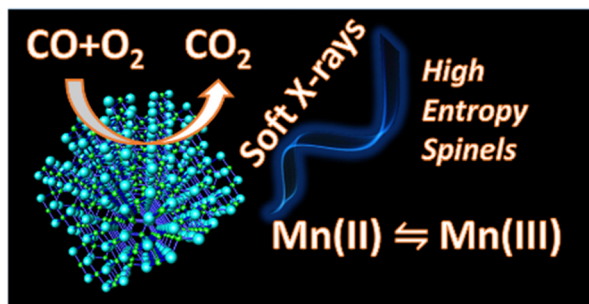
3401



### Pd catalysts doped with B/C atoms in the subsurface: the positive effect of interstitial atoms in regulating the selectivity of acetylene catalytic hydrogenation

Qiao Xie, Xin Liu, Yingying Xing, Liang Huang,\* Wen Lei, Shaowei Zhang and Haijun Zhang\*

3412



### Mechanisms of CO oxidation on high entropy spinels

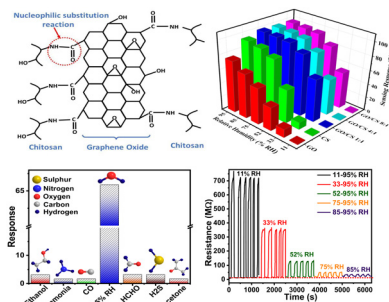
Martina Fracchia, Paolo Ghigna,\* Sara Stolfi, Umberto Anselmi Tamburini, Mauro Coduri, Luca Braglia and Piero Torelli



3420

### High performance humidity sensor based on a graphene oxide–chitosan composite

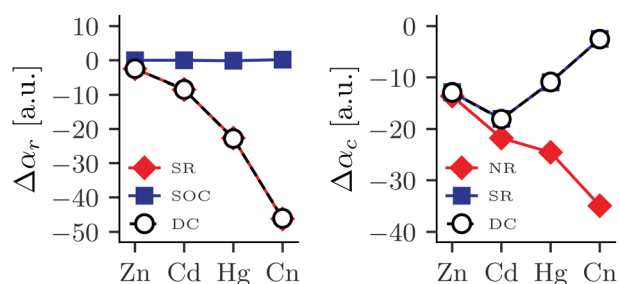
Parvesh Kumari, Ankit Kumar, Aditya Yadav, Ylias Sabri, Samuel J. Ippolito, Dilip. D. Shivagan and Komal Bapna\*



3430

### Relativistic and electron-correlation effects in static dipole polarizabilities for group 12 elements

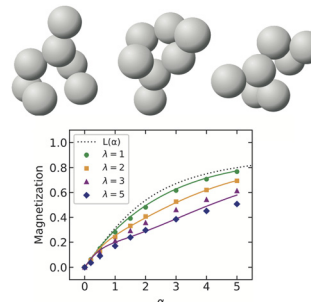
YingXing Cheng



3442

### Magnetization of immobilized multi-core particles with varying internal structures

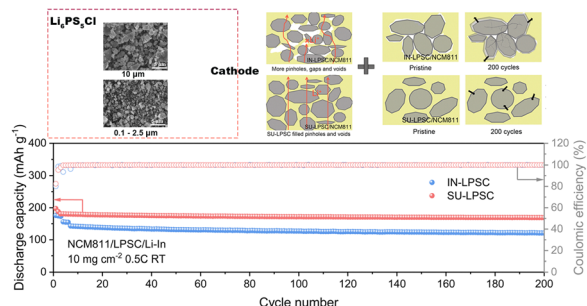
Anna Yu. Solovyova, Elena V. Grohotova, Alexey O. Ivanov and Ekaterina A. Elfimova\*



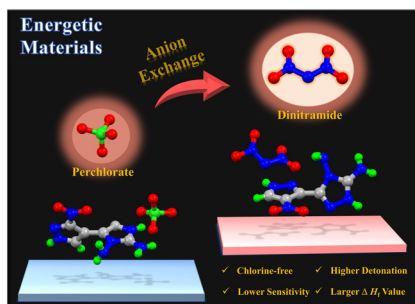
3455

### Sub-micrometer Li<sub>6</sub>PS<sub>5</sub>Cl regulated cathodic Li kinetics in sulfide based all-solid-state batteries

Yuanyuan Lin, Hanzhou Liu, Yaqi Hu, Yang Lu,\* Zongliang Zhang, Yang Liu, Yongle Chen, Kun Zhang, Shuo Yin and Fangyang Liu\*



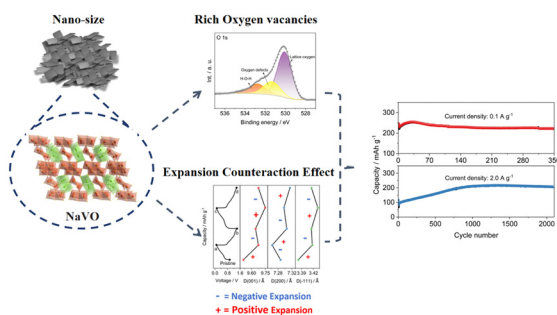
3463



### Dinitramide salts based on nitropyrazole-diaminotriazole hybrid: novel ionic energetic materials with high-energy and low-sensitivity

Jinxiong Cai, Yingqi Xia,\* Hui Zhang, Dongshuai Su, Qi Lai, Ping Yin and Siping Pang\*

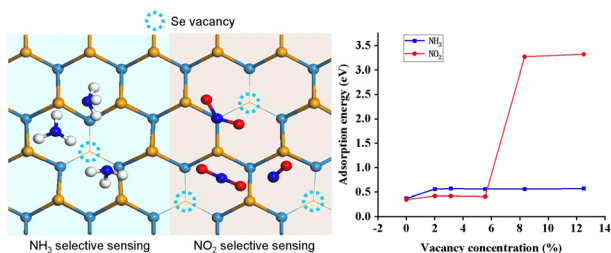
3469



### Expansion counteraction effect assisted vanadate with rich oxygen vacancies as a high cycling stability cathode for aqueous zinc-ion batteries

Xiao-Luan Xie, Yi-Fan Li, Cheng Wang, Da-Wei Gu, Lei Wang, Qiao Qiao, Yang Zou, Zhi-Yuan Yao,\* Lin-Jiang Shen and Xiao-Ming Ren

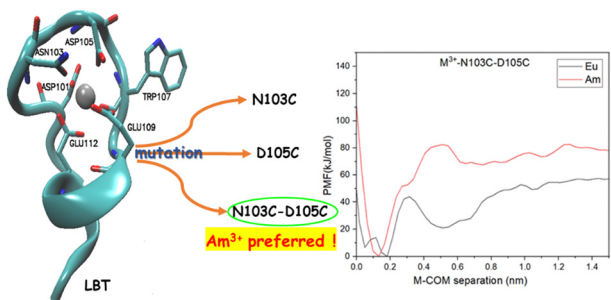
3477



### Selective sensing of NH<sub>3</sub> and NO<sub>2</sub> on WSe<sub>2</sub> monolayers based on defect concentration regulation

Jinghao Zhang, Yunfan Zhang, Fenghui Tian,\* Luxiao Sun, Xiaodong Zhang, Aiping Fu and Mingwei Tian

3486



### Tuning the lanthanide binding tags for preferential actinide chelation: an all atom molecular dynamics study

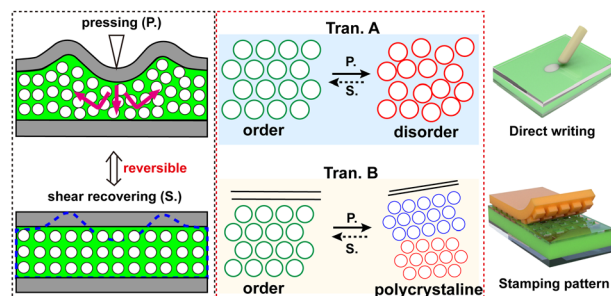
Vijayakriti Mishra,\* Mahesh Sundararajan,\* Arup Kumar Pathak,\* Pramilla D. Sawant and Tusar Bandyopadhyay



3496

## Disappearing and reappearing of structure order in colloidal photonic crystals

Feng Gao, Xinyu Jiang, Junjun Qiu, Tong An, Manyao Zhang, Xiaokun Song, Nan Shi, Xiuhong Li, Tongxiang Fan\* and Qibin Zhao\*



3504

## Synthesis of amino acids in intense laser-irradiated primary amine solutions

Wakako Ishikawa and Shunichi Sato\*

