

IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 27(6) 2855–3512 (2025)



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

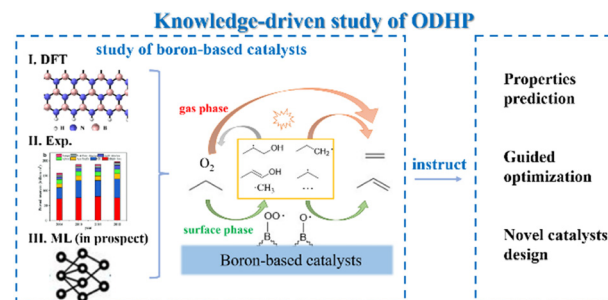
See Daniel Jezierski, José Lorenzana and Wojciech Grochala, pp. 2927–2938. Image reproduced by permission of Daniel Jezierski from *Phys. Chem. Chem. Phys.*, 2025, 27, 2927.

PERSPECTIVE

2874

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

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

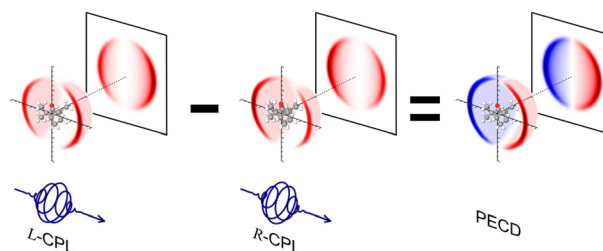


TUTORIAL REVIEW

2888

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

Chris Sparling and Dave Townsend*



ChemComm

**Uncover new possibilities
with outstanding
preliminary research**

**Original discoveries, fuelling
every step of scientific progress**

rsc.li/chemcomm

**Fundamental questions
Elemental answers**

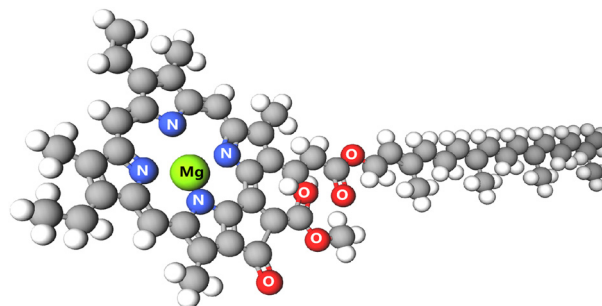


REVIEW

2908

Theory for ultrafast energy transfer in photosynthesis

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

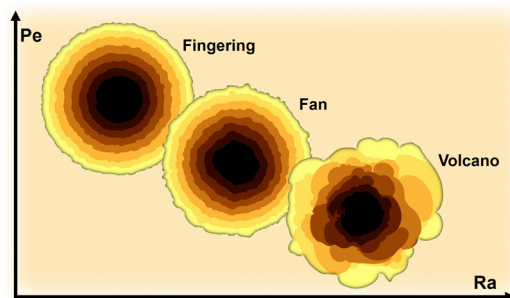


RESEARCH PAPERS

2920

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

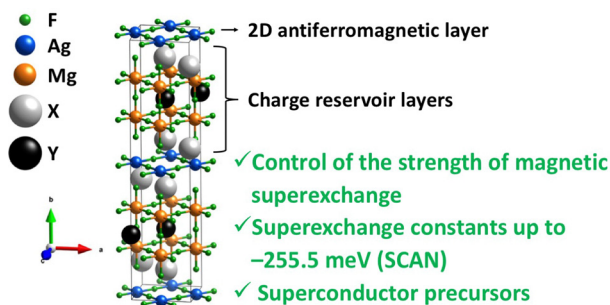
Y. Stergiou,* A. Perrakis, A. De Wit and K. Schwarzenberger*



2927

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

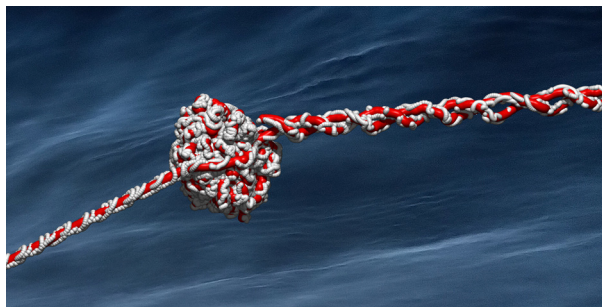
Daniel Jezierski,* José Lorenzana* and Wojciech Grochala*



2939

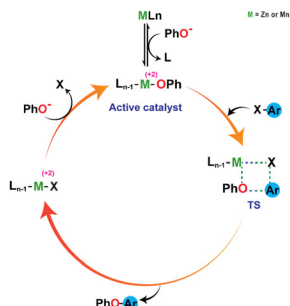
Molecular dynamics of evaporative cooling of water clusters

Martin Klíma, Jiří Janek and Jiří Kolafa*



RESEARCH PAPERS

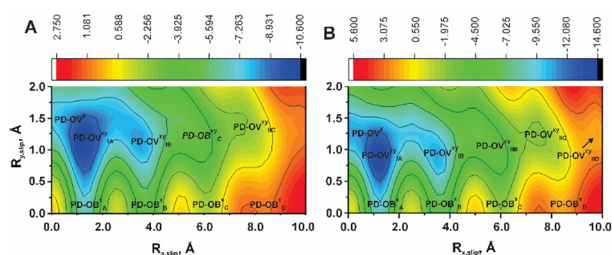
2948



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*

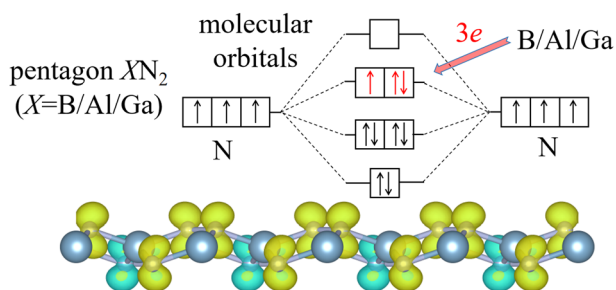
2958



Stack bonding in pentacene and its derivatives

Craig A. Bayse

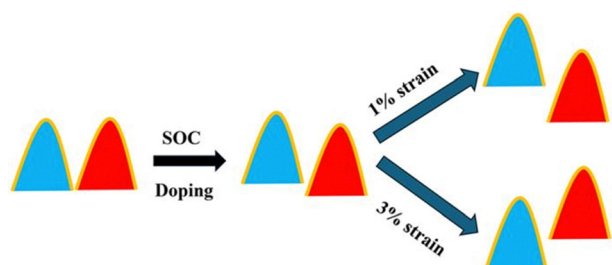
2968



High Néel temperature and magnetism modulation in 2D pentagon-based XN_2 ($X = B, Al$, 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*

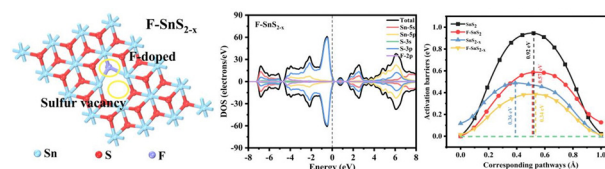


RESEARCH PAPERS

2983

The effect of introducing fluorine doping and sulfur vacancies on SnS_2 as the anode electrode of LIBs: a density functional theory study

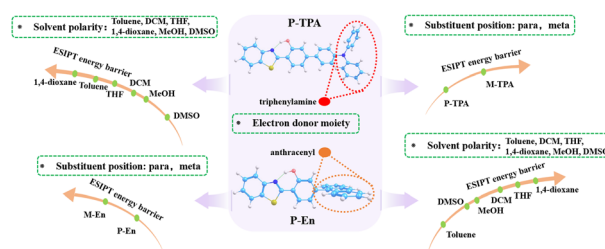
Jiayi Guan, Kaihui Lin, Yanbing Liao, Zhiling Xu, Yuda Lin* and Shenghui Zheng*



2993

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

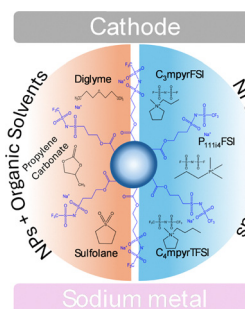
Xiu-Min Liu, Yin Yu, Shu-Ying Xu and Xue-Hai Ju*



3006

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

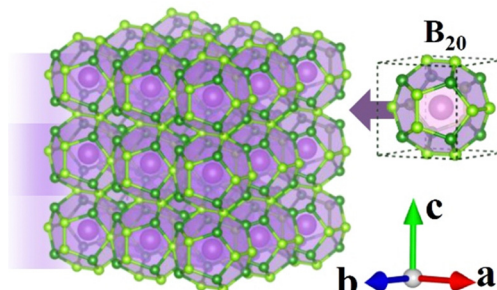
Pierre L. Stigliano,* Antonela Gallastegui, Thomas H. Smith, Luke O'Dell, David Mecerreyes, Cristina Pozo-Gonzalo and Maria Forsyth*



3023

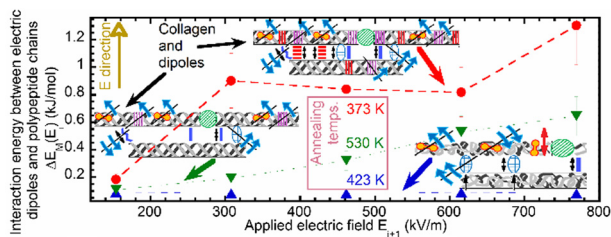
Superconductivity and high hardness in scandium-borides under pressure

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



RESEARCH PAPERS

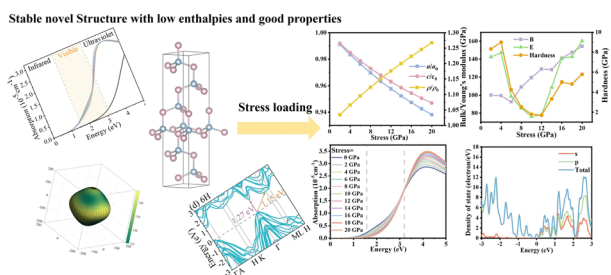
3032



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*

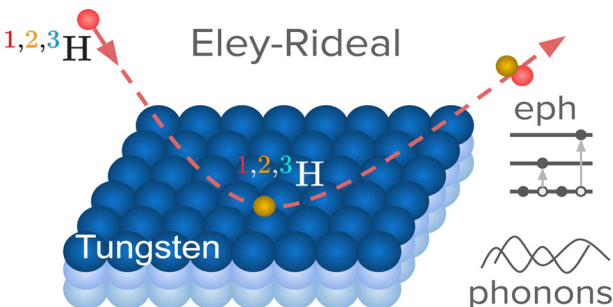
3045



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

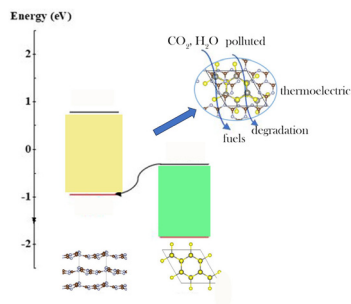
3052



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-C₃N₄/ZnS heterojunction for photocatalytic applications

Elnaz Ranjbakhsh and Mohammad Izadyar*

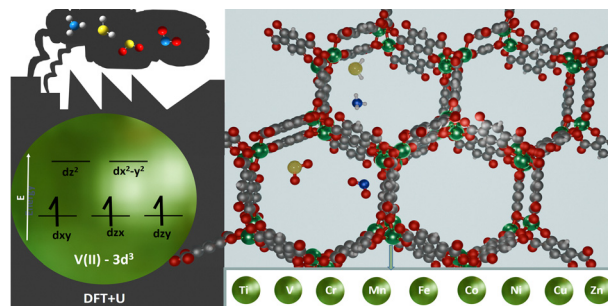


RESEARCH PAPERS

3068

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

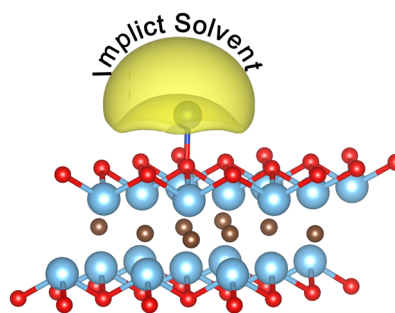
Nazli Jodaeeasl, Shiliang Wang, Anguang Hu and Gilles H. Peslherbe*



3083

Single-atom lead ion adsorption behavior on Ti₂CO₂ MXene under different electrode potentials

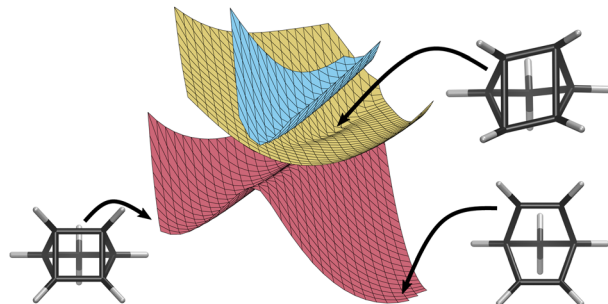
Kechen Li, Yang Ou, Yongzhi Wang, Jianbo Zhang and Yang Zhou*



3089

Electronic structure of norbornadiene and quadricyclane

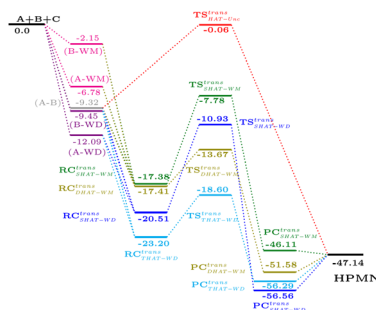
Joseph C. Cooper and Adam Kirrander*



3102

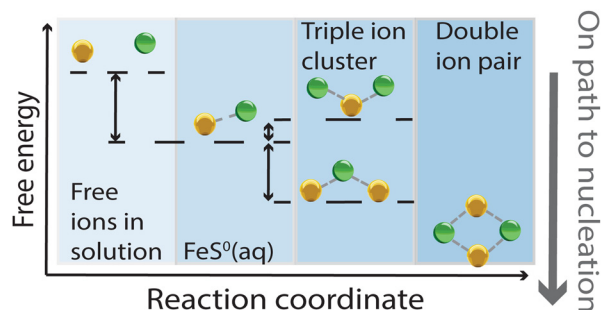
Water as a catalyst in the reaction of nitrous acid (HONO) and Criegee intermediate (CH₂OO)

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



RESEARCH PAPERS

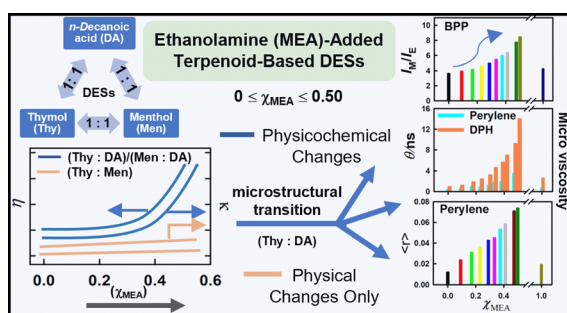
3115



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*

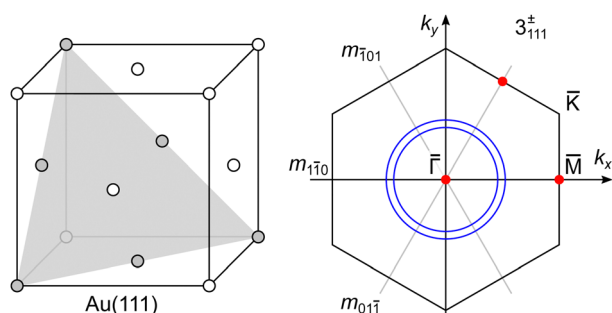
3124



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

Anjali and Siddharth Pandey*

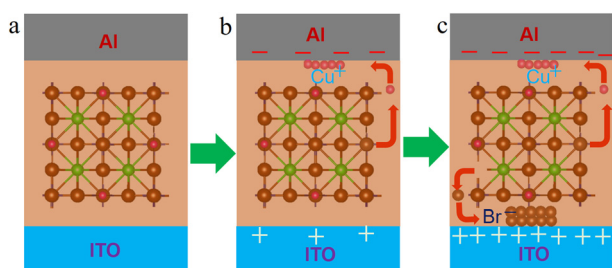
3138



Rashba effect originates from the reduction of point-group symmetries

Koshi Okamura

3150



Air-stable double halide perovskite Cs₂CuBiBr₆: synthesis and memristor application

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

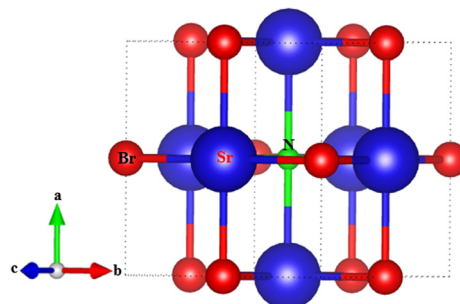


RESEARCH PAPERS

3160

Strain-dependent structural, electronic, mechanical, optical and thermoelectric properties of Sr_3NBr_3 perovskites for solar cell applications

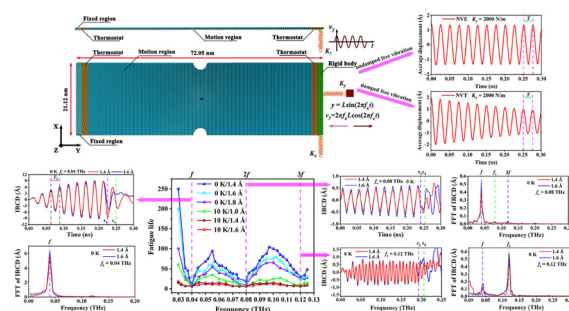
Amina, Naseem Akhter, Salhah Hamed Alrefaee, Anvar Nurmammedov, Mukhlisa Soliyeva, Pervaiz Ahmad, Vineet Tirth, Ali Algahtani, Q. Mohsen, O. Alsaqer, N. M. A. Hadia and Abid Zaman*



3171

Phononic origin of resonance in atomic scale fatigue of MoS_2

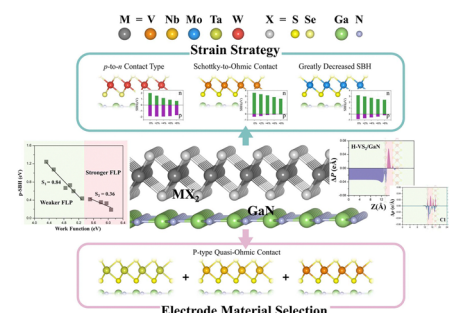
Yun Dong,* Bo Shi, Yi Tao, Xinyi Tang, Jinguang Wang, Futian Yang and Yifan Liu



3185

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

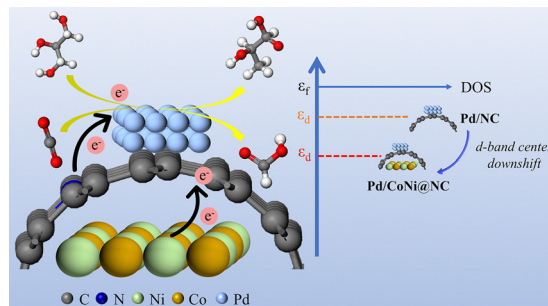
Jing Li, Lei Ao* and Zhihua Xiong*



3198

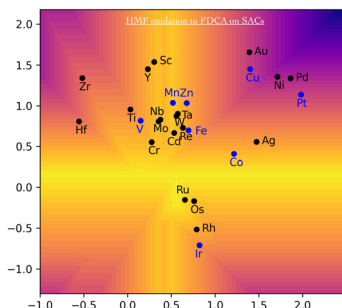
Tuning metal-support interactions in MOF-derived CoNi@NC supported Pd catalysts for efficient hydrogenation of bicarbonate using glycerol as a hydrogen donor

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



RESEARCH PAPERS

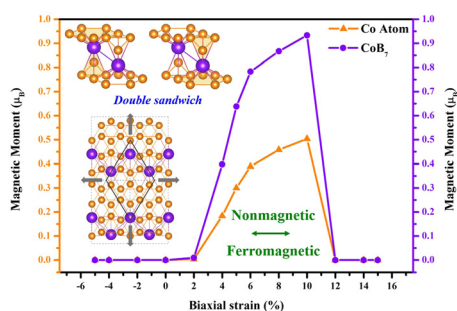
3206



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*

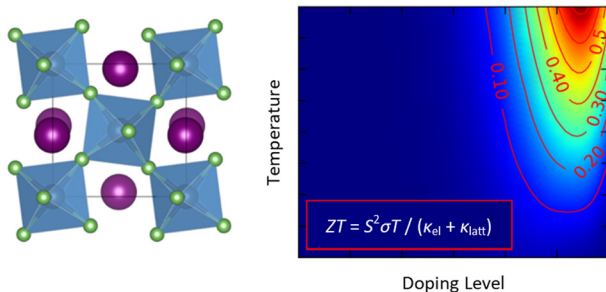
3217



Two-dimensional inverse double sandwich CoB₇: strain-induced non-magnetic to ferromagnetic transition

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

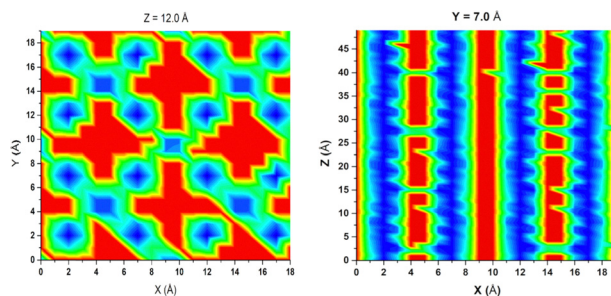
3230



Thermoelectric properties of the low-spin lanthanide cobaltate perovskites LaCoO₃, PrCoO₃, and NdCoO₃ from first-principles calculations

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

3243



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*

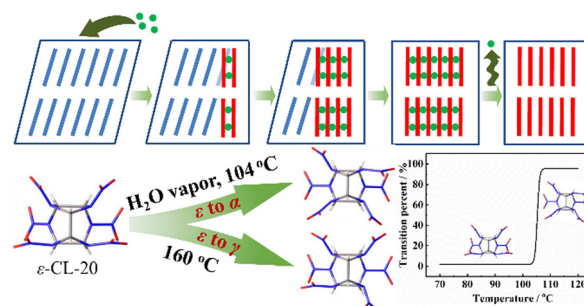


RESEARCH PAPERS

3253

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

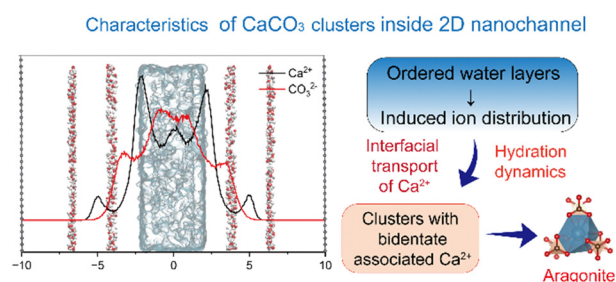
Ya Guo,* Xueting Cai, Fangbao Jiao, Zhicheng Guo, Qi Huang and Qi Zhang*



3263

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

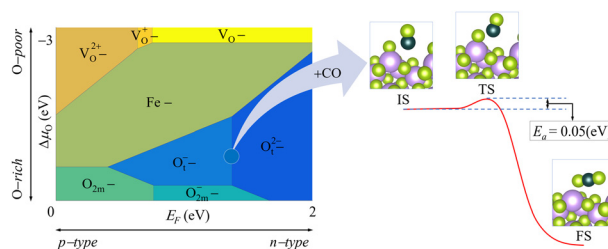
Jia-Ying Li, Rui-Tian Ma, Shi-Qi Zheng, Tian Xia and Hai-Bo Yi*



3278

Revealing the catalytic oxidation mechanism of CO on $\alpha\text{-Fe}_2\text{O}_3$ surfaces: an *ab initio* thermodynamic study

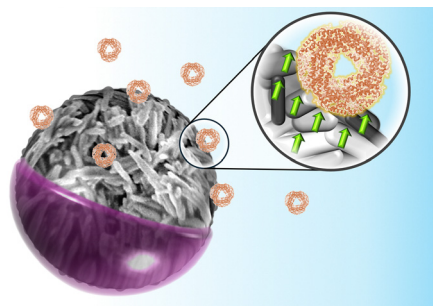
Yun-Hyok Song, Yun-Hyok Kye,* Myong-Il Pang, Yong-Min Ho, Hyon-Chol Choe, Chol-Jun Yu* and Chol-Yong Ri



3291

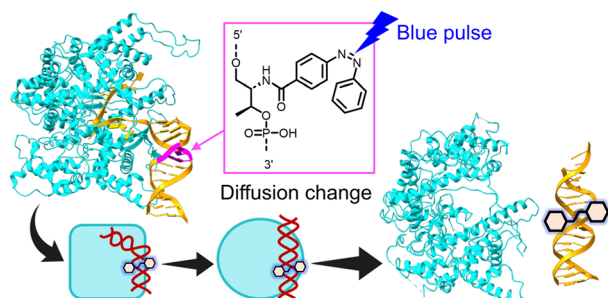
Probing spin effects in phycocyanin using Janus-like ferromagnetic microparticles

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



RESEARCH PAPERS

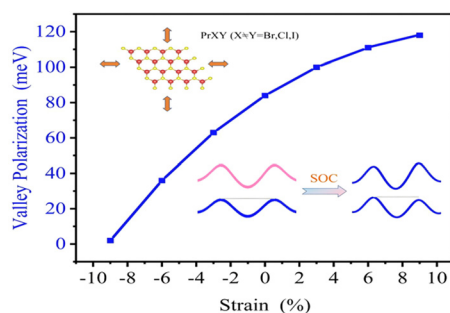
3302



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

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

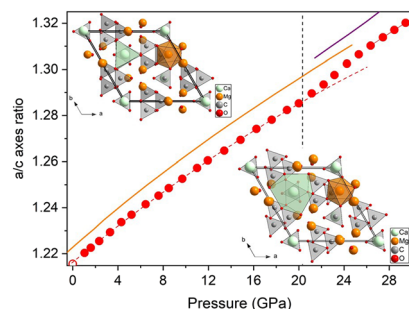
3313



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*

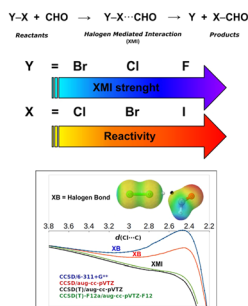
3320



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, Dario J. R. Duarte* and Victor M. Rayón*

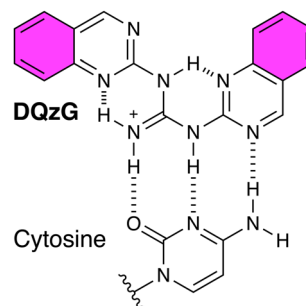


RESEARCH PAPERS

3341

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

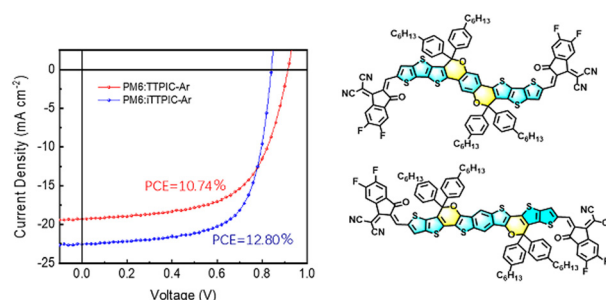
Eitaro Murakami, Tomonori Shibata,* Megumi Tomemori, Gota Kawai and Kazuhiko Nakatani*



3351

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

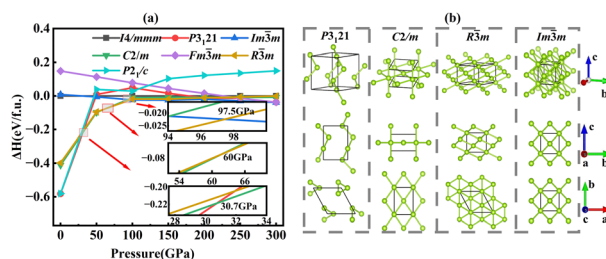
Jiamo Zhou, Xinying Ruan, Yufan Zhu, Ziqi Han, Jingyao Kong, Dan He* and Fuwen Zhao*



3357

Phase transition and superconductivity of selenium under pressure

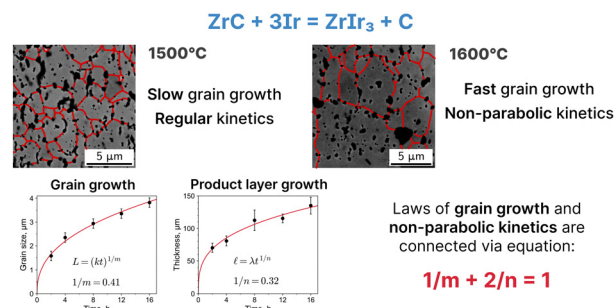
Enci Zuo, Yingying Chen,* Gang Jiang, Liang Zhao and Jiguang Du*



3363

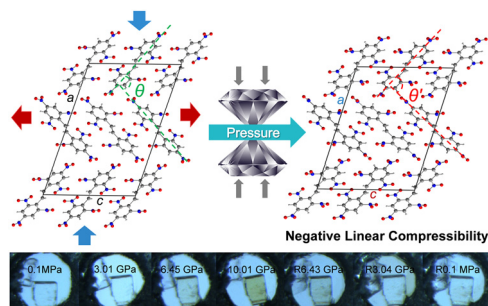
How grain structure evolution affects the kinetics of a solid-state reaction: a case of interaction between iridium and zirconium carbide

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



RESEARCH PAPERS

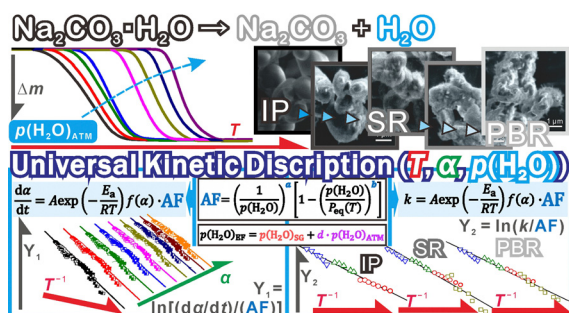
3375



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*

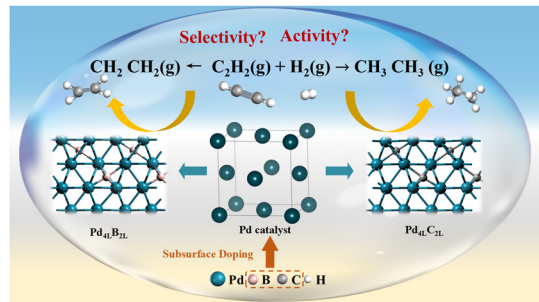
3384



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*

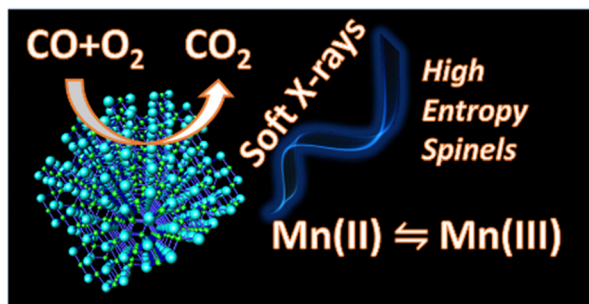
3401



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

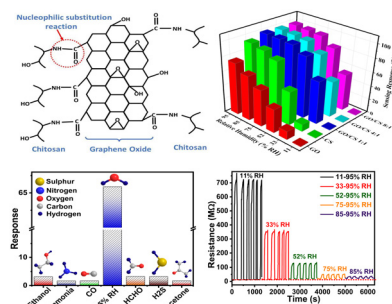


RESEARCH PAPERS

3420

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

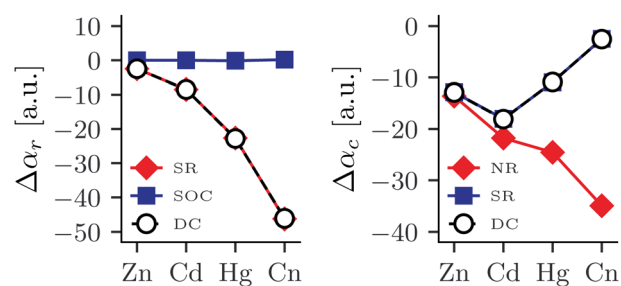
Parvesh Kumari, Ankit Kumar, Aditya Yadav, Ylias Sabri, Samuel J. Ippolito, Dilip. D. Shivagan and Komal Bapna*



3430

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

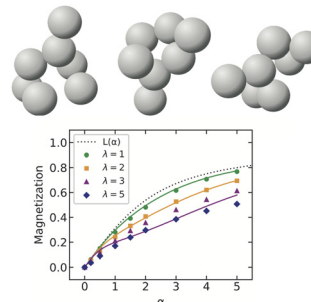
YingXing Cheng



3442

Magnetization of immobilized multi-core particles with varying internal structures

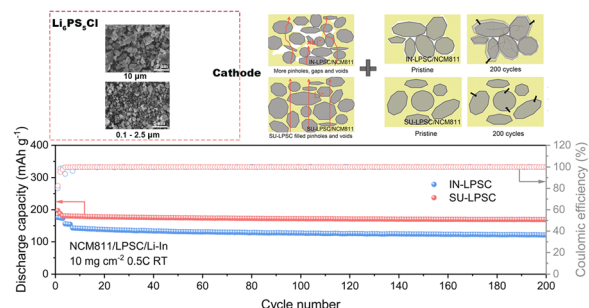
Anna Yu. Solovyova, Elena V. Grohotova, Alexey O. Ivanov and Ekaterina A. Elfimova*



3455

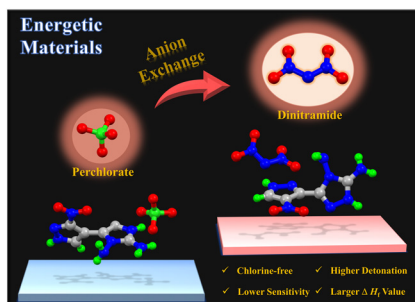
Sub-micrometer Li₆PS₅Cl regulated cathodic Li kinetics in sulfide based all-solid-state batteries

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



RESEARCH PAPERS

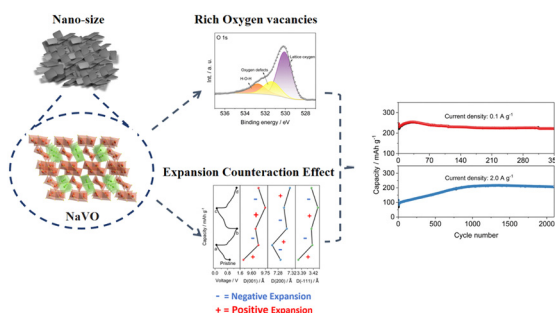
3463



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*

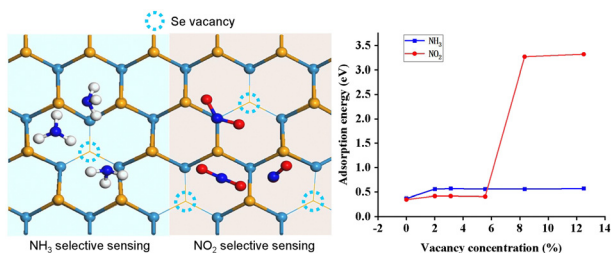
3469



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

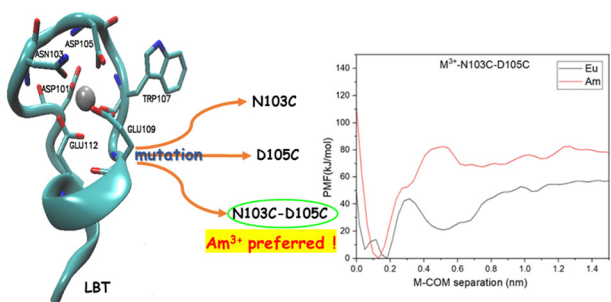
3477



Selective sensing of NH₃ and NO₂ on WSe₂ 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

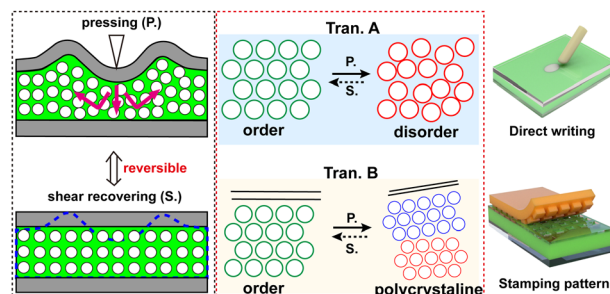


RESEARCH PAPERS

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*

