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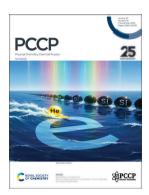
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#### Cover

See Yasuko Koshiba, Kenji Ishida et al., pp. 21871-21877. Image reproduced by permission of Yasuko Koshiba from Phys. Chem. Chem. Phys., 2025, **27**, 21871.



#### Inside cover

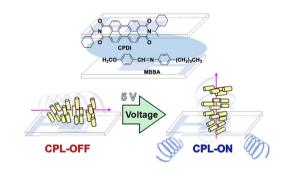
See Feng Wang, Lan Jiang et al., pp. 21878-21885. Image reproduced by permission of Feng Wang from Phys. Chem. Chem. Phys., 2025, **27**, 21878. Artwork generated using Google Gemini.

# COMMUNICATION

## 21867

Electric field-induced circularly polarised luminescence switching in chiral nematic liquid crystals with negative dielectric anisotropy

Daiya Suzuki, Kosuke Kaneko and Yoshitane Imai\*

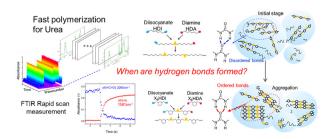


#### RESEARCH PAPERS

## 21871

In situ observation of polyurea formation by rapid-scan time-resolved infrared spectroscopy

Yasuko Koshiba,\* Satoshi Atsumi, Tatsuya Fukushima, Shohei Horike and Kenji Ishida\*





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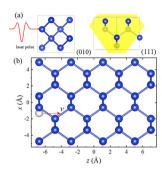
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#### 21878

# Electron stopping power of $\alpha$ -particles in silicon regulated by ultrashort pulse lasers

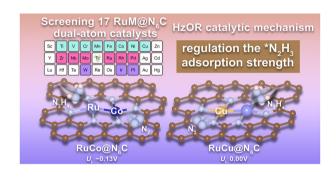
Ya-Ting Sun, Xiao-Ning Yang, Xin Shen, Feng Wang\* and Lan Jiang\*



#### 21886

# Boosting hydrazine electrooxidation on Ru-coordinated heteronuclear double metal atom catalysts

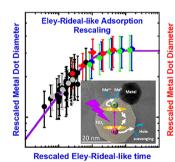
Zhengfeng Zhang, Zhonghui Gao, Yangin Liang, Hui Jiang, Zhaoyang Li, Zhenduo Cui, Enzuo Liu, Shengli Zhu and Wence Xu\*

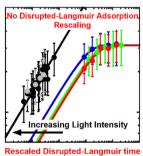


## 21895

Discriminating adsorption mechanisms in liquid-phase photocatalysis via high-intensity laser-induced metallic nanodot deposition on TiO<sub>2</sub> anatase

Fenghuan Zhao, Qingguo Bai, Eugenie Pariente, Marie-Helene Delville\* and Jean-Pierre Delville\*

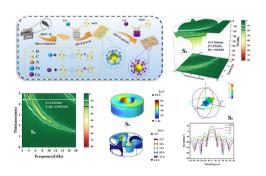




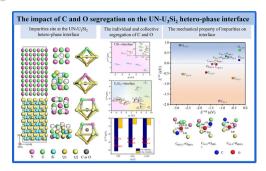
#### 21909

Optimization of electromagnetic parameters and efficient wave-absorbing performance of FeSiAl@bimetallic MOF composite wave-absorbing materials constructed by an in situ growth method

Yuzhi Wang, Xiaopeng Qi,\* Yifeng Hu, Changcai Chen, Zhengxing Li, Weiwei Dong, Quan Fang and Lei Wang\*



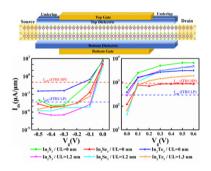
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# Carbon and oxygen segregation at the UN(010)/ U<sub>3</sub>Si<sub>2</sub>(001) interface: insights from first-principles calculations

Liu Xi, Yuanyuan Wang,\* Jiajun Zhao and Jijun Zhao

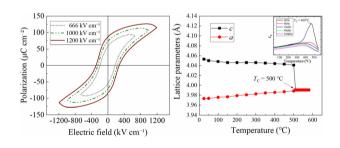
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# 5 nm Gate length field-effect transistors based on monolayer $\alpha$ -In<sub>2</sub>X<sub>3</sub> (X = S, Se, Te)

Yun-Ya Zhong, Jian-Qing Dai,\* Jin Yuan, Da-Wei Deng and Miao-Wei Zhao

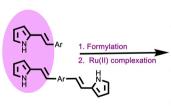
#### 21949



# Simultaneously achieving large ferroelectric polarization and high $T_C$ in sol-gel deposited PbTiO<sub>3</sub>-based perovskite thin films

Mengqi Ye, Jin Liu, Duo Wang, Zhao Pan,\* Fengyi Zhou, Xubin Ye, Huajie Luo, Nianpeng Lu, Yunzhong Chen, Ruilong Wang and Youwen Long\*

#### 21956



- · series of pyrrolecontaining frameworks
- · iterative increase in conjugation
- · third harmonic generation

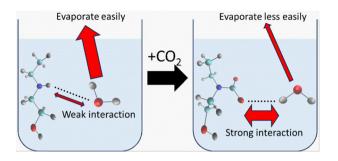
# Third-order nonlinear optical properties of a series of pyrroles and dipyrroles featuring $\pi$ -conjugated substituents and linkers

Elisha Bennett, Adil Alkaş, Roberto M. Diaz-Rodriguez, Jacob W. Campbell, Luke A. Ferguson, Michael J. Cotnam, Richard Cisek, Alison Thompson\* and Danielle Tokarz\*

#### 21970

# Thermodynamic properties of water in aqueous amine solutions studied by energy-representation method

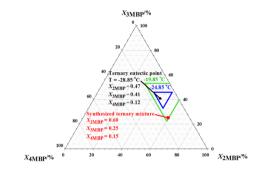
Yuki Yokoyama, Keiji Yasuda and Tsuyoshi Yamaguchi\*



#### 21982

# Mixture of methylbiphenyls as potential liquid organic hydrogen carriers

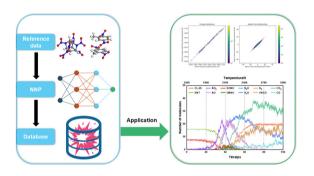
Byeong Soo Shin, Seon Hwa Baek, Joori Jung, Chang Won Yoon, Sang Kyu Kwak,\* Won-Sik Han\* and Jeong Won Kang\*



# 21994

# A neural network potential model for CL-20/DNT high-energy material: thermal stability regulation and decomposition mechanism

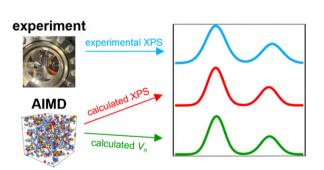
Yifan Zhang, Hongyang Liu, Meiheng Lv,\* Huaxin Liu, Yinhua Ma, Fangjian Shang, Jianyong Liu\* and Wenze Li\*



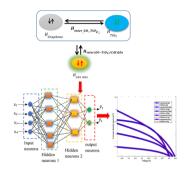
#### 22004

# Core-level binding energies describe electrostatic potentials at nuclei for ionic liquids

Frances K. Towers Tompkins, Ekaterina Gousseva, Roger A. Bennett, Ricardo Grau-Crespo and Kevin R. J. Lovelock\*



#### 22013



Interfacial quantum dynamics and Al-driven engineering of CdS quantum dot-sensitized solar cells based on GO-TiO2 nanocomposite photoanode

Salaheddine Mansouri,\* Mokhtar Hjiri, Nejmeddine Yahyaoui and Fahrettin Yakuphanoglu

The isomerization mechanisms of nitrenes CF<sub>3</sub>CXN at temperatures below 300 K.

 $X = CH_2$ : cyclization is always the dominant mechanism.

X = NH: cyclization reverse-cyclization (> 200 K).

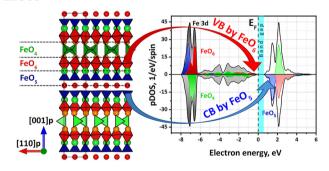
X = O: Curtius reaction (< 150 K);

cyclization --- Curtius reaction (> 150 K).

A theoretical study of the isomerization mechanisms of nitrenes  $CF_3CXN$  (X = O, NH,  $CH_2$ ): competing intersystem crossing reactions driven by heavy-atom quantum tunneling

Ciliang Xie\* and Zhen Hua Li

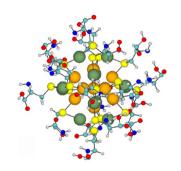
## 22039



Highly anisotropic electronic properties of the GdBa<sub>2</sub>Ca<sub>2</sub>Fe<sub>5</sub>O<sub>13</sub> oxide: a DFT+U study of a potential air electrode for solid oxide fuel cells

Boris Politov,\* Igor Shein and Susana Garcia-Martin\*

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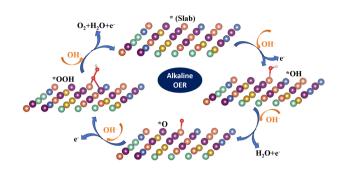
Thermal stability of L-cysteine-protected Au<sub>25</sub> clusters: interplay between melting and ligand desorption

Michael A. Short, Alexey V. Verkhovtsev, Theodoros Pavloudis, Richard E. Palmer\* and Andrey V. Solov'yov

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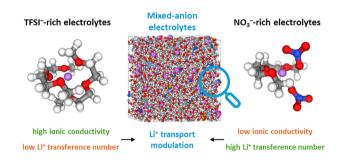
Prediction of oxygen evolution reaction activity of FCC\_CoCuFeNiPd and CoCuFeNiRu multi-principal element alloys based on sublattice preference of constituent atoms and the site preference of intermediates

Longju Su, Hehua Que, Cheng Qian, Xiaogiong Zhang, Xingyu Chen, Rong Chen, Jiansen Wen\* and Bo Wu\*



Strongly vs. weakly associating anions: transport-structure relationship in LiTFSI-LiNO<sub>3</sub> electrolytes

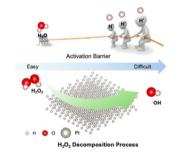
Ervin Rems,\* Tim Šlosar, Sara Drvarič Talian, Matej Huš, Robert Dominko and Alessandra Serva\*



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Questioning the role of adsorbed H in H<sub>2</sub>O<sub>2</sub> decomposition on Pt(111) for the electrocatalytic green Fenton process

Chentao Xu, Ji Li and Zhizhang Shen\*

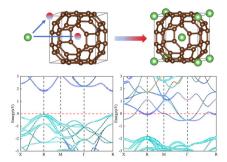


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# Electronic properties of ThC<sup>-</sup> and ThC

Isuru R. Ariyarathna

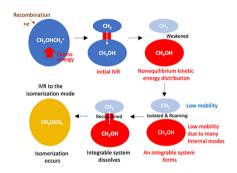
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# Superconductivity induced by element doping in C<sub>48</sub> fullerene at ambient pressure

Weiguo Sun, Dexin Mu, Xiaofeng Li,\* Simin Li and Feng Peng\*

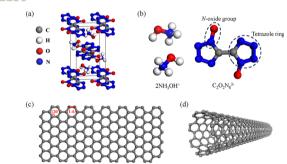
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# Roaming-controlled formation of dimethyl ether and methanol: role of nonequilibrium dynamics and integrability

Toshiaki Matsubara

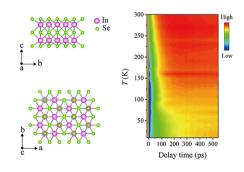
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# Enhancing thermal transport in TKX-50 energetic materials: the role of graphene orientation and molecular interactions

Shuping Zhang, Xiao Xu,\* Xunjian Zhang, Liqian Song and Xu Jia\*

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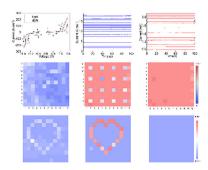
# Hot carrier decay dynamics of van der Waals room temperature ferroelectric α-In<sub>2</sub>Se<sub>3</sub>

Chunlian Li, Borong Cong, Jiajun Cao, Weizheng Liang\* and Bingsuo Zou\*

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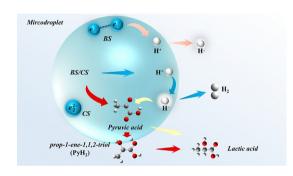
Investigation of the NbO<sub>x</sub> phase change self-selective memristor-based photoelectric synapse features

Tongyu Wang, Haofeng Ran,\* Jiahao Guo, Wenhua Wang, Xiaofang Hu, Changrong Liao, Bai Sun, Yuejun Kang\* and Guangdong Zhou\*



Competing pathways of spontaneous two-electron reduction of pyruvic acid in water microdroplets

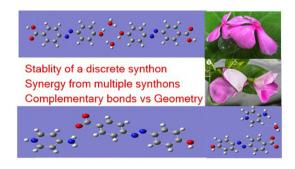
Jiaqi Cao and Zhenyu Li\*



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Are supramolecular synthons stable as discrete units? Results from a series of salts of 4-(4-hydroxyphenylazo)benzoic acid and its derivatives with aminopyridines

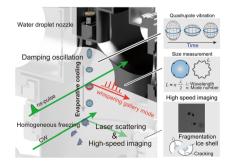
Munendra Pal Singh, Abhinav Hazarika and Jubaraj B. Baruah\*



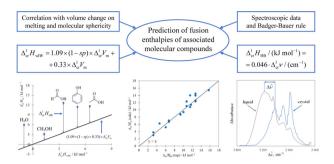
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# Kinematic and thermodynamic studies on water micro-droplets supercooled in a vacuum

Takefumi Handa, Masashi Arakawa, Masato Yamaguchi, Takuya Horio and Akira Terasaki\*

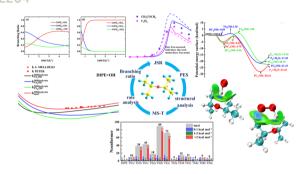


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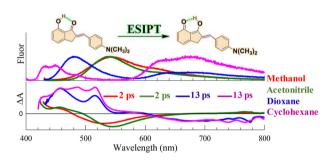
Hydrogen bonding and van der Waals forces contributions to the melting enthalpy: insights from volumetric and spectroscopic data

Andrey A. Sokolov,\* Boris N. Solomonov and Mikhail I. Yagofarov



Theoretical and kinetic studies of H-abstraction from diisopropyl ether by key radicals: implications for combustion chemistry

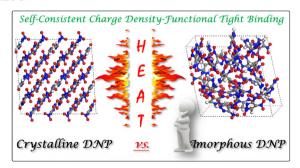
Xingzhi Wang, Jiuning He, \* Xue Zou, Jianhua Li, Lei Chen, Yanhao Duan, Jia Li, Changhua Zhang and Deliang Chen



Planarity-induced enhancement of excited-state proton transfer and near-infrared emission in conjugated N,N-dimethylamino cyclic chalcone derivatives: a combined photophysical and theoretical investigation

Balgees S. Al-Saadi, Ahmed H. Ismail, Younis Baqi,\* John Husband\* and Osama K. Abou-Zied\*

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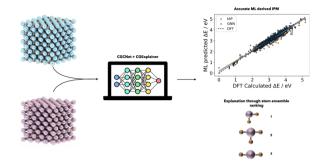
Quantum mechanics insights into the early pyrolysis mechanism of 3,4-dinitro-1*H*-pyrazole in the amorphous model

Shuangfei Zhu, Shufen Zheng, Wenjun Rao, Yi Yang,\* Ruijun Gou\* and Shuhai Zhang

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# Explainable GNN-derived structure-property relationships in interstitial-alloy materials

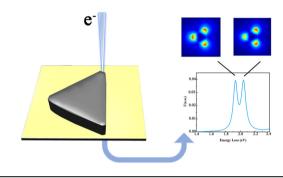
Eduardo Aguilar-Bejarano, Luis Arrieta, Mauricio Gutiérrez, Ender Özcan, Simon Woodward, Grazziela Figueredo\* and J. Ignacio Borge\*



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# Study of plexcitons in a metal nanotriangle-WS<sub>2</sub> composite system using electron energy loss spectroscopy

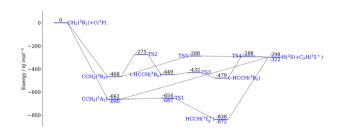
Rongyue Yao, Yuan Zhang, Changlin Zheng and Luxia Wang\*



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# The $C(^{3}P) + CH_{2}(^{3}B_{1})$ reaction: accurate electronic structure calculations and kinetics for astrochemical modeling

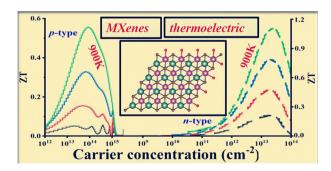
Michel Lorin, S. Rasoul Hashemi and Gunnar Nyman\*



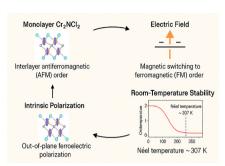
# 22268

A theoretical study of the thermoelectric properties of two-dimensional surface-functionalized MXene materials ScYCTT' (T = OH, H; T' = H, F)

Long-Fei Cui, Wen-Li Chang,\* Qing-Chao Liu, Tao Wang, Xiao-Ping Wei and Xiao-Ma Tao



22280



# Electric-field-induced magnetic switching in a monolayer MXene Cr2NCl2 with intrinsic electronic polarization

Jianwei Wei, Jian Chen, Kexin Chen, Yaohui Yin, Ai Wang and Chao Xin\*