

IN THIS ISSUE

ISSN 1463-9076 CODEN PPCPFQ 27(41) 21853–22290 (2025)



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

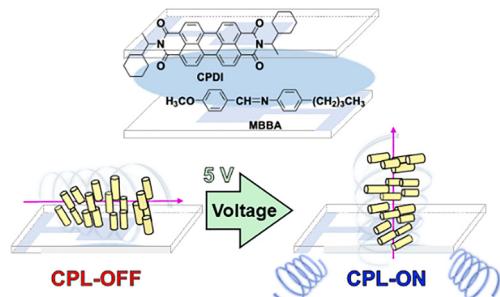
See Feng Wang, Lan Jiang *et al.*, pp. 21878–21885. Image reproduced by permission of Feng Wang from *Phys. Chem. Chem. Phys.*, 2025, 27, 21878. Artwork generated using Google Gemini.

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*

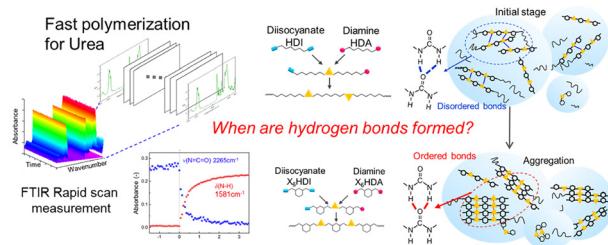


RESEARCH PAPERS

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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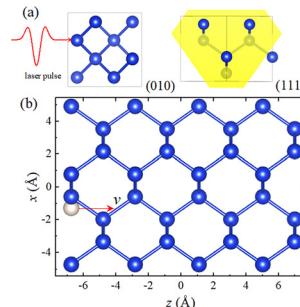


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21878

Electron stopping power of α -particles in silicon regulated by ultrashort pulse lasers

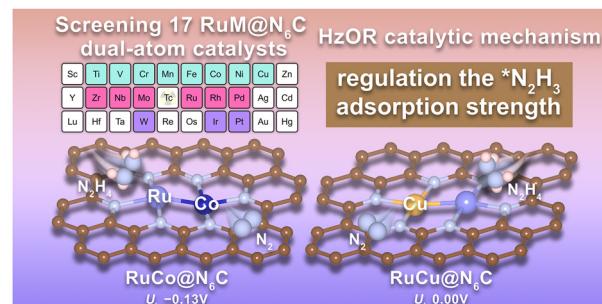
Ya-Ting Sun, Xiao-Ning Yang, Xin Shen, Feng Wang* and Lan Jiang*



21886

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

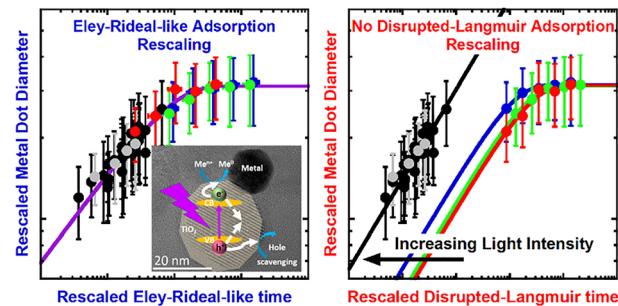
Zhengfeng Zhang, Zhonghui Gao, Yanqin Liang, Hui Jiang, Zhaoyang Li, Zhenduo Cui, Enzuo Liu, Shengli Zhu and Wence Xu*



21895

Discriminating adsorption mechanisms in liquid-phase photocatalysis via high-intensity laser-induced metallic nanodot deposition on TiO_2 anatase

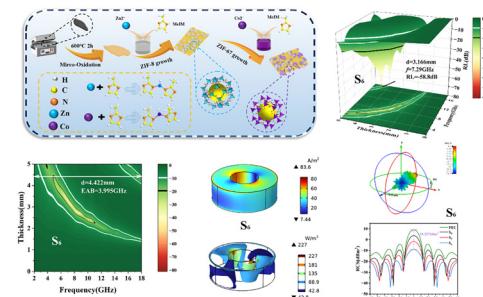
Fenghuan Zhao, Qingguo Bai, Eugenie Pariente, Marie-Helene Delville* and Jean-Pierre Delville*



21909

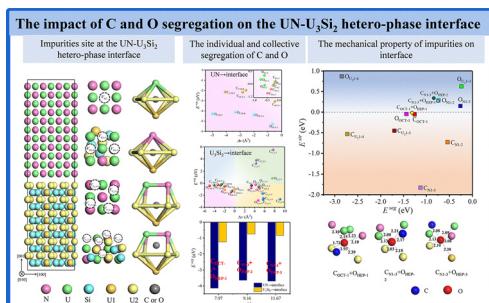
Optimization of electromagnetic parameters and efficient wave-absorbing performance of FeSiAl@bimetallic MOF composite wave-absorbing materials constructed by an *in situ* growth method

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



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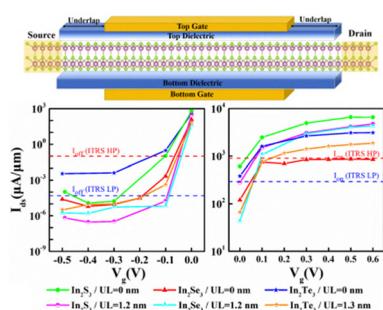
21923



Carbon and oxygen segregation at the UN(010)/UN₃Si₂(001) interface: insights from first-principles calculations

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

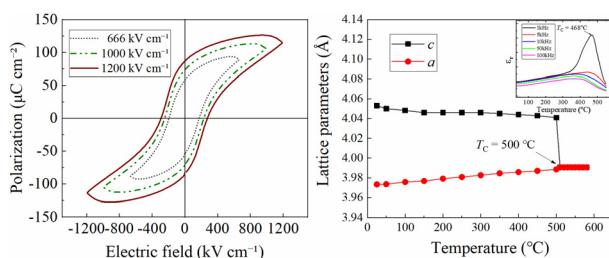
21937



5 nm Gate length field-effect transistors based on monolayer α -In₂X₃ (X = S, Se, Te)

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

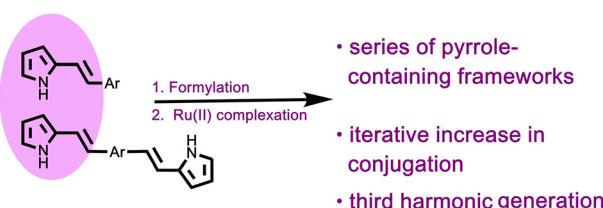
21949



Simultaneously achieving large ferroelectric polarization and high T_c in sol-gel deposited PbTiO_3 -based perovskite thin films

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

21956



Third-order nonlinear optical properties of a series of pyrroles and dipyrroles featuring π -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*

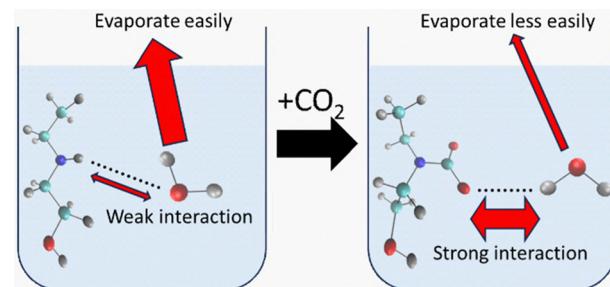


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21970

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

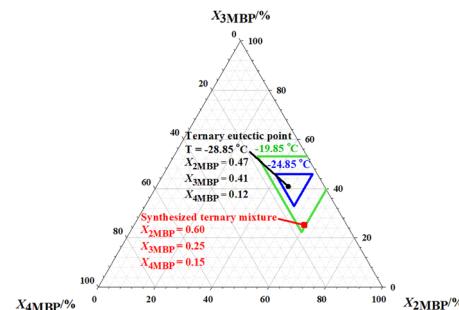
Yuki Yokoyama, Keiji Yasuda and Tsuyoshi Yamaguchi*



21982

Mixture of methylbiphenyls as potential liquid organic hydrogen carriers

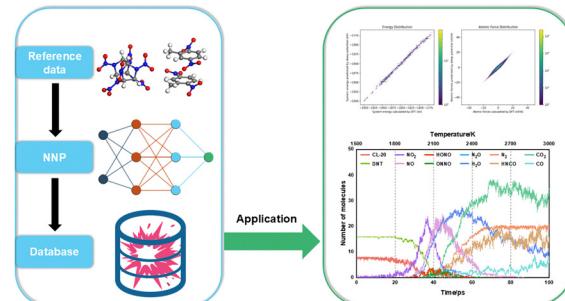
Byeong Soo Shin, Seon Hwa Baek, Joori Jung, Chang Won Yoon, Sang Kyu Kwak,* Won-Sik Han* and Jeong Won Kang*



21994

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

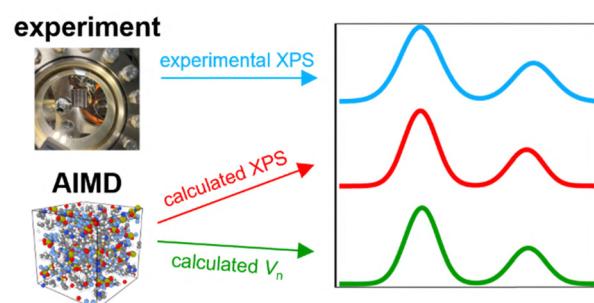
Yifan Zhang, Hongyang Liu, Meiheng Lv,* Huaxin Liu, Yinhua Ma, Fangjian Shang, Jianyong Liu* and Wenzhe Li*



22004

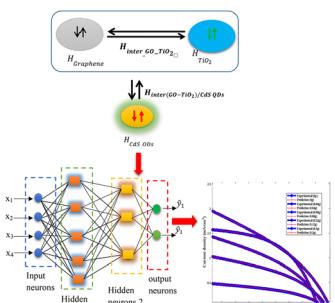
Core-level binding energies describe electrostatic potentials at nuclei for ionic liquids

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



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22013

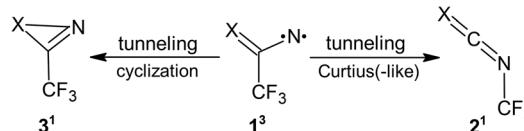


Interfacial quantum dynamics and AI-driven engineering of CdS quantum dot-sensitized solar cells based on GO-TiO₂ nanocomposite photoanode

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

22026

The isomerization mechanisms of nitrenes CF₃CXN at temperatures below 300 K.

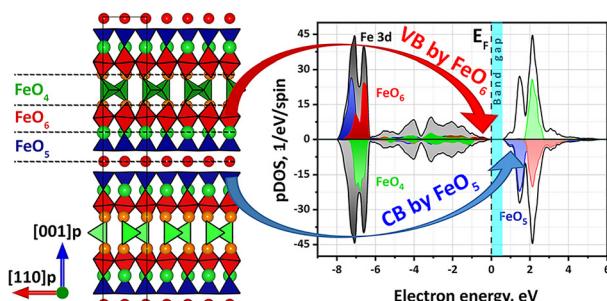


X = CH₂: cyclization is always the dominant mechanism.
 X = NH: cyclization ← reverse-cyclization (> 200 K).
 X = O: Curtius reaction (< 150 K);
 cyclization ← reverse-cyclization → Curtius reaction (> 150 K).

A theoretical study of the isomerization mechanisms of nitrenes CF₃CXN (X = O, NH, CH₂): competing intersystem crossing reactions driven by heavy-atom quantum tunneling

Ciliang Xie* and Zhen Hua Li

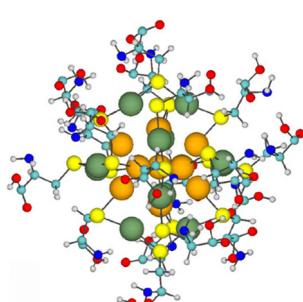
22039



Highly anisotropic electronic properties of the GdBa₂Ca₂Fe₅O₁₃ oxide: a DFT+U study of a potential air electrode for solid oxide fuel cells

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

22054



Thermal stability of L-cysteine-protected Au₂₅ clusters: interplay between melting and ligand desorption

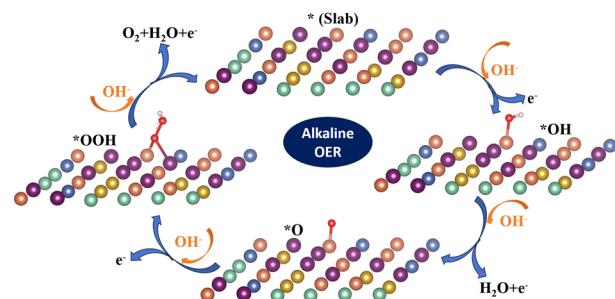
Michael A. Short, Alexey V. Verkhovtsev, Theodoros Pavloudis, Richard E. Palmer* and Andrey V. Solov'yov

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22064

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

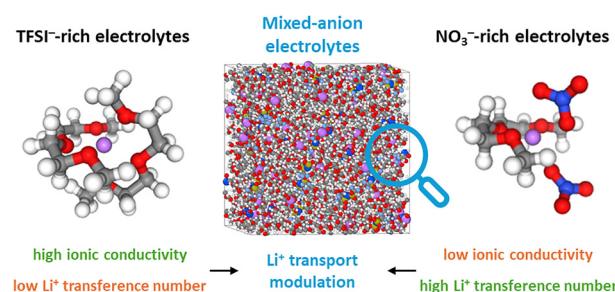
Longju Su, Hehua Que, Cheng Qian, Xiaoqiong Zhang, Xingyu Chen, Rong Chen, Jiansen Wen* and Bo Wu*



22082

Strongly vs. weakly associating anions: transport–structure relationship in LiTFSI–LiNO₃ electrolytes

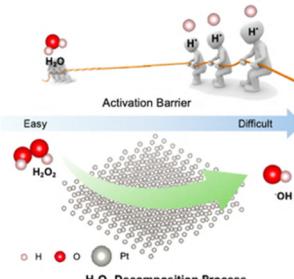
Ervin Rems,* Tim Šlosar, Sara Drvarič Talian, Matej Huš, Robert Dominko and Alessandra Serva*



22093

Questioning the role of adsorbed H in H₂O₂ decomposition on Pt(111) for the electrocatalytic green Fenton process

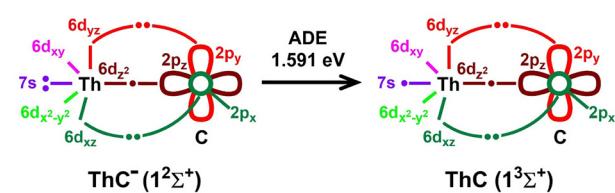
Chentao Xu, Ji Li and Zhizhang Shen*



22103

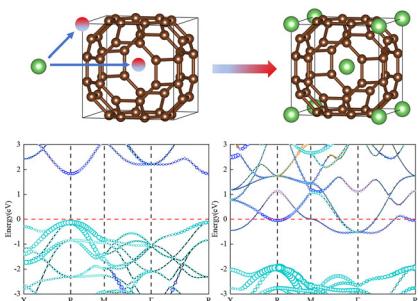
Electronic properties of ThC[−] and ThC

Isuru R. Ariyarathna



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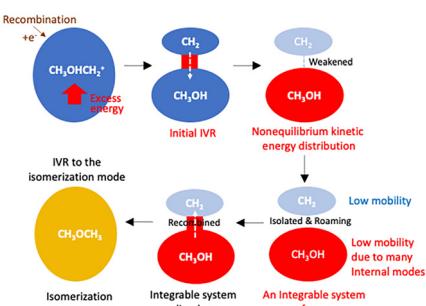
22114



Superconductivity induced by element doping in C_{48} fullerene at ambient pressure

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

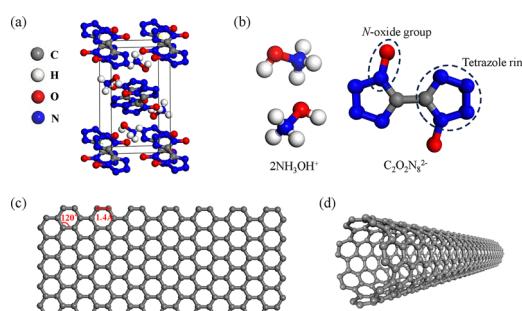
22121



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

Toshiaki Matsubara

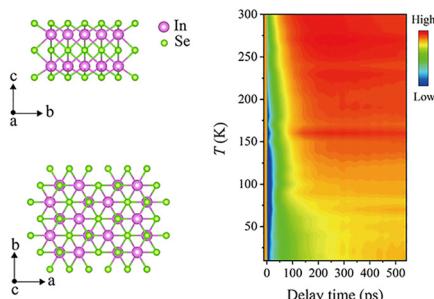
22139



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*

22148



Hot carrier decay dynamics of van der Waals room temperature ferroelectric α -In₂Se₃

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

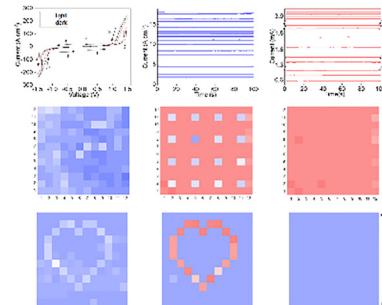


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22156

Investigation of the NbO_x phase change self-selective memristor-based photoelectric synapse features

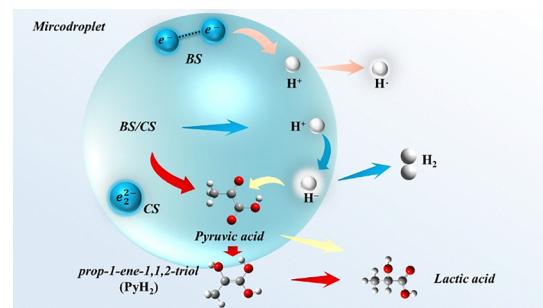
Tongyu Wang, Haofeng Ran,* Jiahao Guo, Wenhua Wang, Xiaofang Hu, Changrong Liao, Bai Sun, Yuejun Kang* and Guangdong Zhou*



22165

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

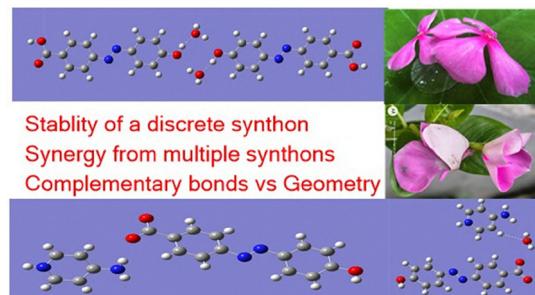
Jiaqi Cao and Zhenyu Li*



22173

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

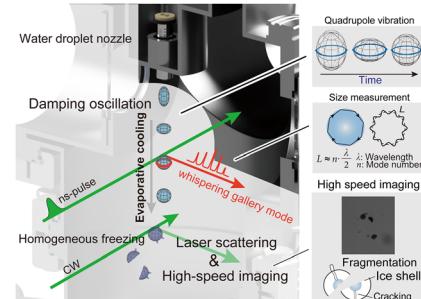
Munendra Pal Singh, Abhinav Hazarika and Jubaraj B. Baruah*



22187

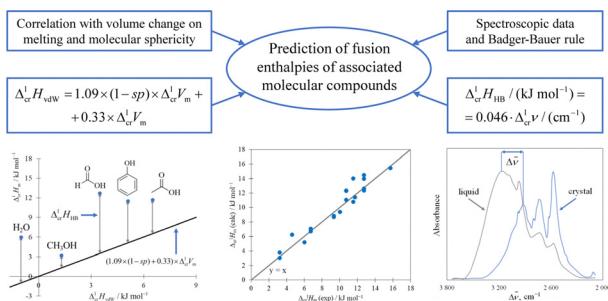
Kinematic and thermodynamic studies on water micro-droplets supercooled in a vacuum

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



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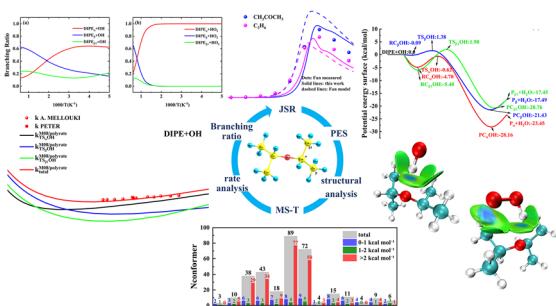
22196



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

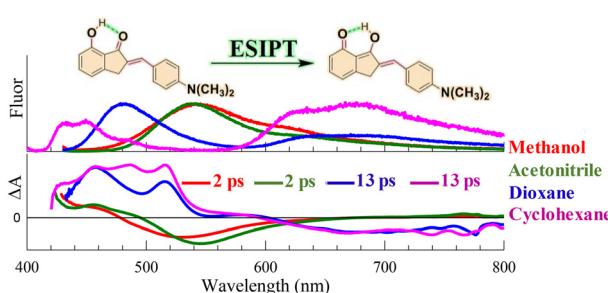
22204



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

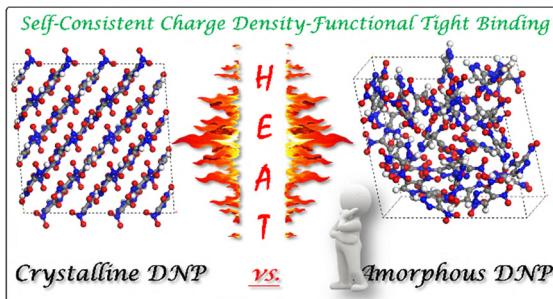
22220



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

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

22230



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

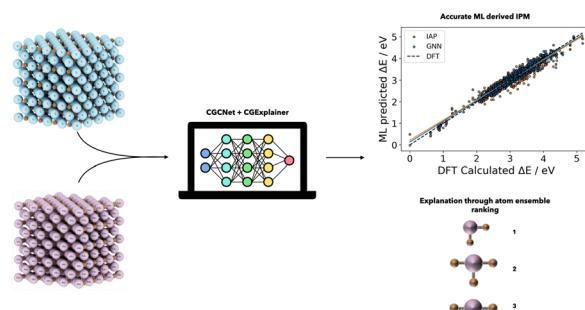


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22240

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

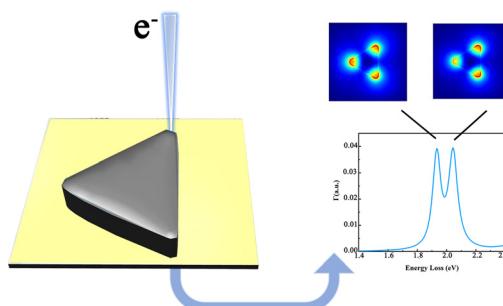
Eduardo Aguilar-Bejarano, Luis Arrieta, Mauricio Gutiérrez, Ender Özcan, Simon Woodward, Grazziela Figueiredo* and J. Ignacio Borge*



22251

Study of plexcitons in a metal nanotriangle–WS₂ composite system using electron energy loss spectroscopy

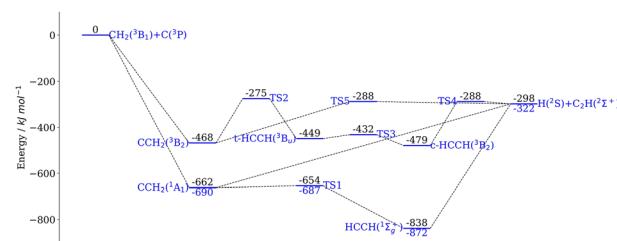
Rongyue Yao, Yuan Zhang, Changlin Zheng and Luxia Wang*



22258

The C(³P) + CH₂(³B₁) reaction: accurate electronic structure calculations and kinetics for astrochemical modeling

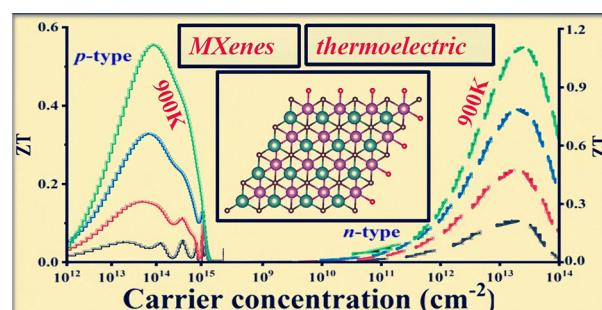
Michel Lorin, S. Rasoul Hashemi and Gunnar Nyman*



22268

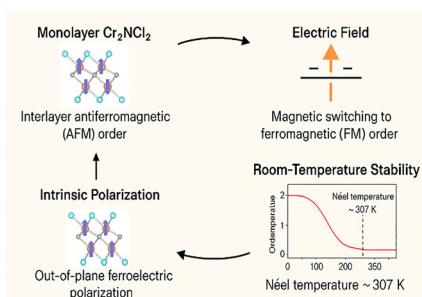
A theoretical study of the thermoelectric properties of two-dimensional surface-functionalized MXene materials ScYCTT' (T = OH, H; T' = H, F)

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



RESEARCH PAPERS

22280



Electric-field-induced magnetic switching in a monolayer MXene Cr_2NCl_2 with intrinsic electronic polarization

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

