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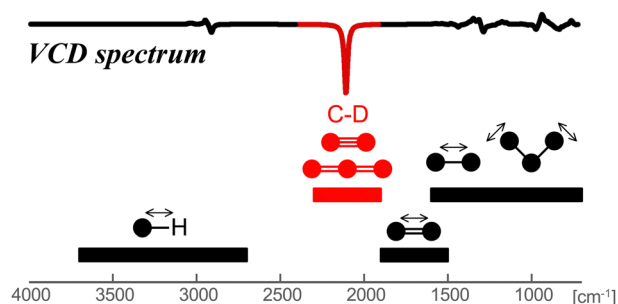
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*Phys. Chem. Chem. Phys.*,  
2023, 25, 28581.

## PERSPECTIVE

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### Vibrational circular dichroism spectroscopy in the C–D, $X\equiv Y$ , and $X=Y=Z$ stretching region

Tohru Taniguchi\* and Davidson Obinna Agbo

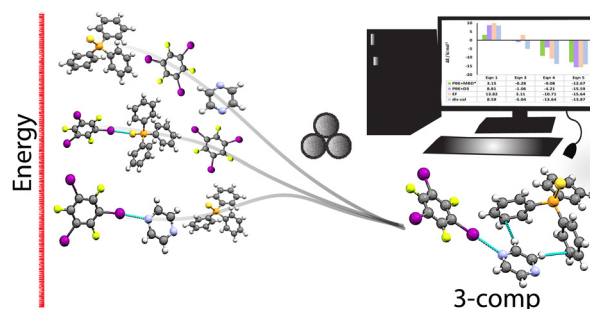


## COMMUNICATION

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### Elucidating mechanochemical reactivity of a ternary halogen-bonded cocrystal system by computational and calorimetric studies

Lavanya Kumar, Sibananda G. Dash, Katarina Leko, Damian Trzybiński, Nikola Bregović,\* Dominik Cincić\* and Mihails Arhangeliskis\*



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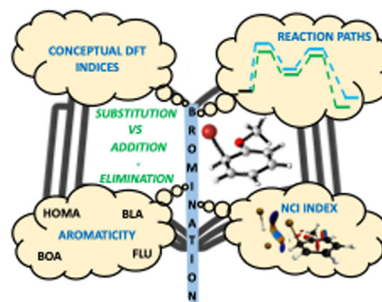


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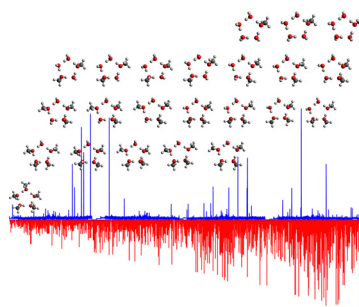
Xavier Deraet, Eline Desmedt, Ruben Van Lommel, Veronique Van Speybroeck and Frank De Proft\*



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# Supersonic jet chirped pulse microwave spectroscopy of ring-like methanol : water pentamers

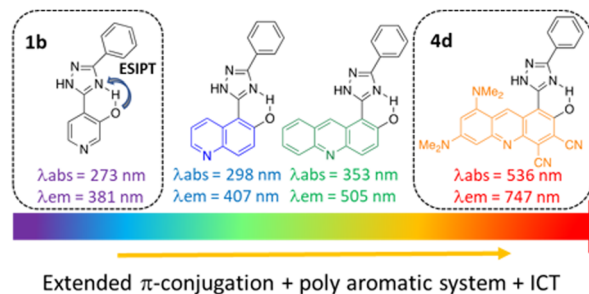
E. M. Mastin,\* S. E. Dutton\* and G. A. Blake\*



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# In silico design of bio-marker detection fluorescent probes

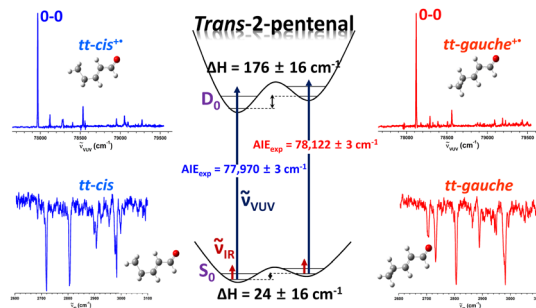
Andrea Echeverri,\* Candice Botuha, Tatiana Gómez, Eleonora Luppi, Julia Contreras-García and Carlos Cárdenas



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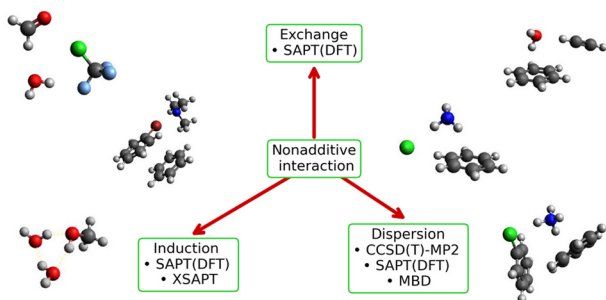
# Conformational diversity and environmental implications of *trans*-2-pentenal

Sung Man Park and Chan Ho Kwon\*



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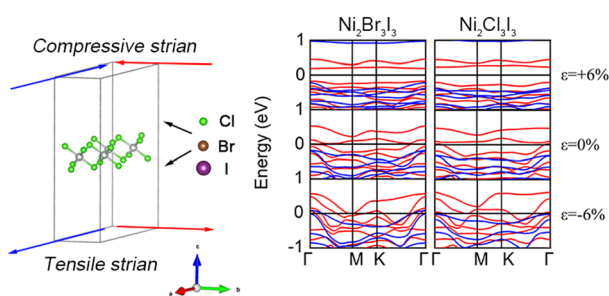
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### Accurate three-body noncovalent interactions: the insights from energy decomposition

Sharon A. Ochieng and Konrad Patkowski\*

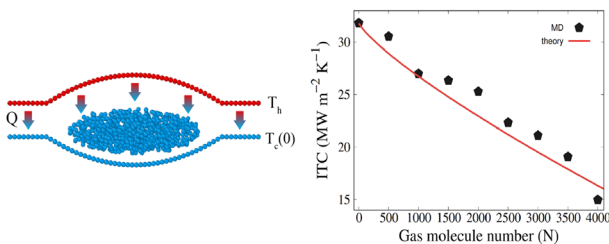
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### Dirac semimetallic Janus Ni-trihalide monolayer with strain-tunable magnetic anisotropy and electronic properties

Bo Chen, Xiaocha Wang\* and Wenbo Mi\*

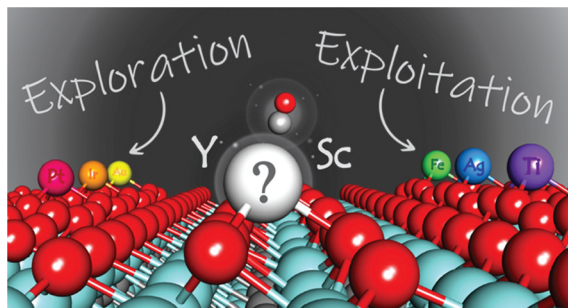
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### Nanobubble-induced significant reduction of the interfacial thermal conductance for few-layer graphene

Zhao-Xia Qu and Jin-Wu Jiang\*

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Kajjana Boonpalit, Jiramet Kinchagawat, Chanatkran Prommin, Sarana Nutanong\* and Supawadee Namuangruk\*



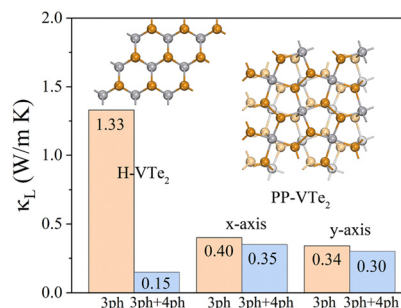


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### The effect of four-phonon interaction on phonon thermal conductivity of hexagonal $\text{VTe}_2$ and puckered pentagonal $\text{VTe}_2$

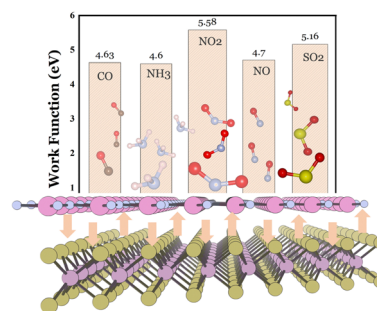
Dan Jin, Pan Zhang, Zhixue Tian, Zhenhua Zhang, Youyuan Yuan, Yong Liu, Zhihong Lu and Rui Xiong\*



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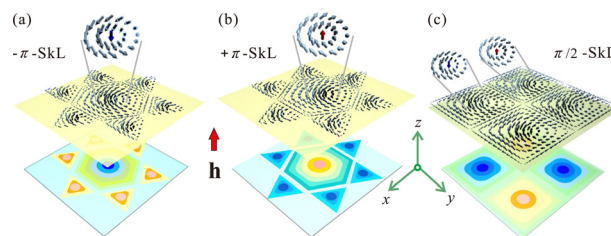
Jaafar Abdul-Aziz Mehrez, Xiyu Chen, Min Zeng,\* Jianhua Yang, Nantao Hu, Tao Wang, Ruili Liu, Lin Xu, Yorexis González-Alfaro and Zhi Yang\*



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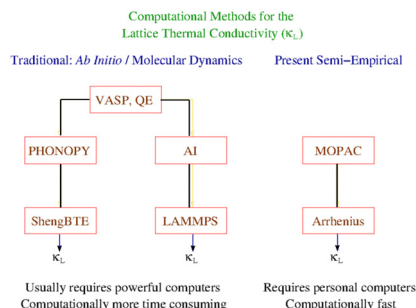
Andrey O. Leonov



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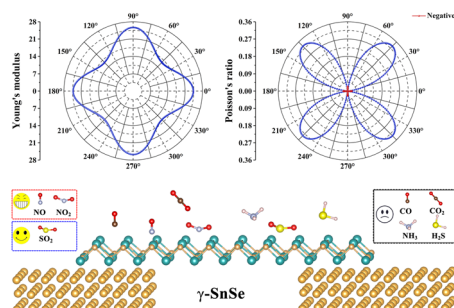
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R. M. Tromer,\* I. M. Felix, L. F. C. Pereira, M. G. E. da Luz,\* L. A. Ribeiro Junior\* and D. S. Galvão



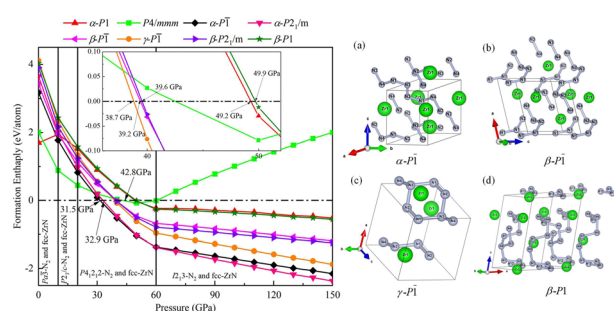
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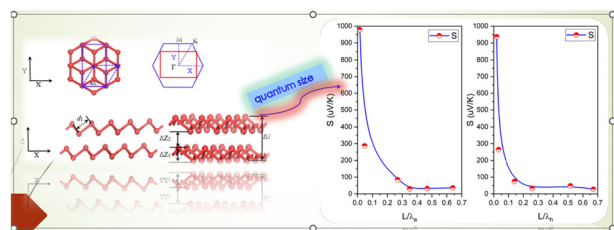
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Pressure-induced novel  $\text{ZrN}_4$  semiconductor materials with high dielectric constants: a first-principles study

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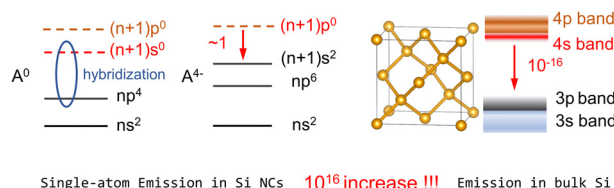
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## Effects of quantum size on the thermoelectric properties of bismuth

Changyi Wu,\* Lei Sun and Jinchen Han

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## Single-atom infrared emission in doped silicon nanocrystals

Feilong Wang, Qiongrong Ou and Shuyu Zhang\*

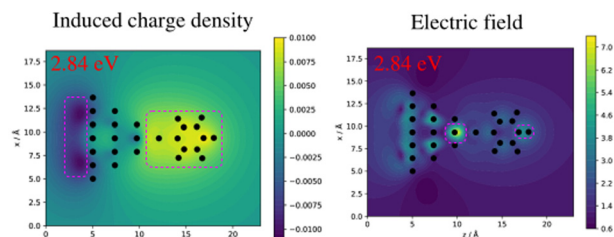


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**Plasmon induced hot carrier generation in a pyridine@Au20 composite**

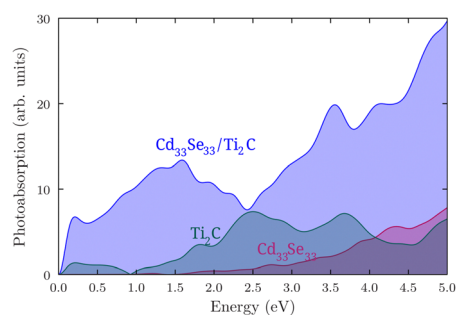
Junais Habeeb Mokkath\*



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**Interface plasmon damping in the  $\text{Cd}_{33}\text{Se}_{33}/\text{Ti}_2\text{C}$  MXene heterostructure**

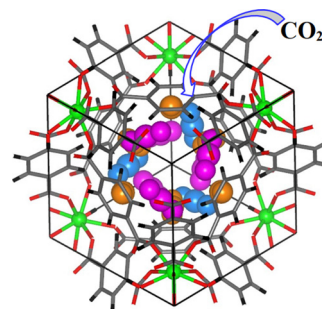
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**Carbon dioxide adsorption to UiO-66: theoretical analysis of binding energy and NMR properties**

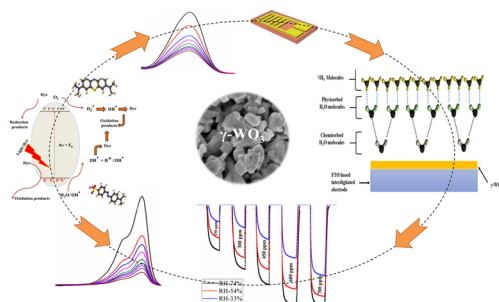
Michiko Atsumi, Jia-Jia Zheng, Erik Tellgren, Shigeyoshi Sakaki\* and Trygve Helgaker\*



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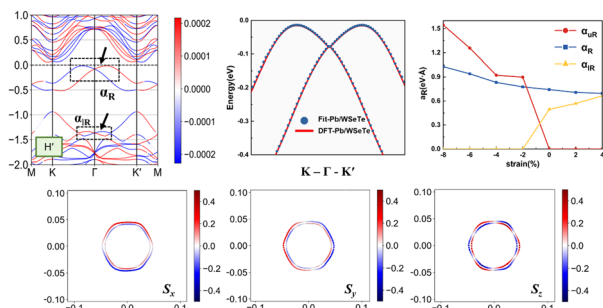
**Tailored mesoporous  $\gamma\text{-WO}_3$  nanoplates: unraveling their potential for highly sensitive  $\text{NH}_3$  detection and efficient photocatalysis**

Shubham Tripathi,\* Jyoti Yadav, Atul Kumar, Raj Kamal Yadav, Pratima Chauhan, Ravindra Kumar Rawat and Satyam Tripathi



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### The tunable anisotropic Rashba spin–orbit coupling effect in Pb-adsorbed Janus monolayer WSeTe

Can Yang, Jia Li,\* Xiaoli Liu and Congling Bai

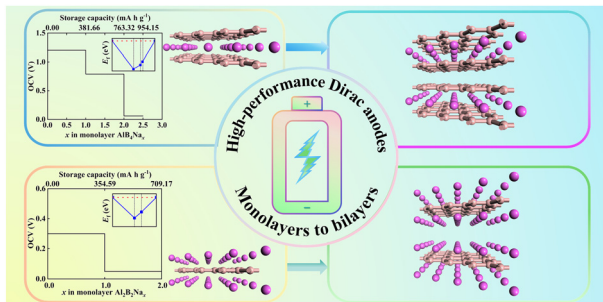
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### A theoretical study of novel orthorhombic group-IVB nitride halide monolayers for photocatalytic overall water splitting

Jiali Wang, Jiajun Lu, Xiuwen Zhao, Guichao Hu, Xiaobo Yuan, Siyun Qi\* and Junfeng Ren\*

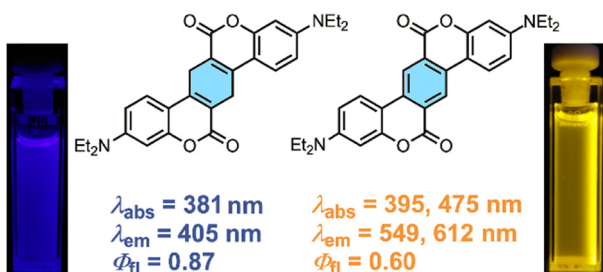
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### Two-dimensional AlB<sub>4</sub>/Al<sub>2</sub>B<sub>2</sub>: high-performance Dirac anode materials for sodium-ion batteries

Ru-Feng Zou, Xiao-Juan Ye,\* Xiao-Hong Zheng, Ran Jia and Chun-Sheng Liu\*

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### Strongly emitting, centrosymmetric, ladder-type bis-coumarins with crankshaft architecture

G. Dinesh Kumar, Yu-Chan Liao, Rashid Nazir, Marzena Banasiewicz, Pi-Tai Chou\* and Daniel T. Gryko\*

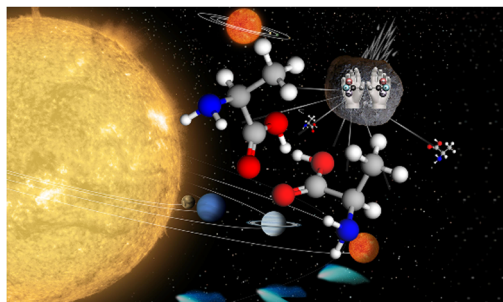


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**Enantiodetermining processes in the synthesis of alanine, serine, and isovaline**

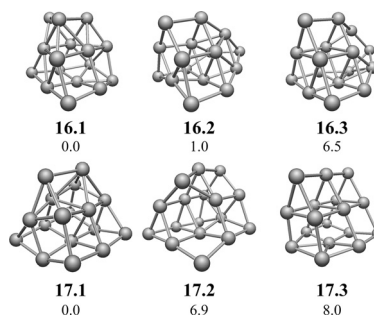
Qingli Liao, Peng Xie and Zhao Wang\*



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**On the structure and electronic properties of  $Pt_n$  clusters: new most stable structures for  $n = 16-17$** 

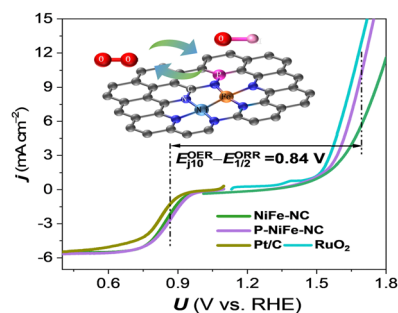
José Manuel Guevara-Vela, Tomás Rocha-Rinza, Peter L. Rodríguez-Kessler\* and Alvaro Muñoz-Castro\*



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**P-doped binary Ni/Fe–N–C for enhanced oxygen electrocatalysis performance**

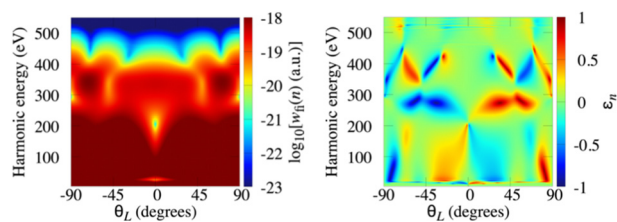
Hongrui Jia, Xiangshe Meng, Yan Lin, Danni Wang, Guoqiang Li\* and Guoxin Zhang\*



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**High-order harmonic generation by aligned homonuclear diatomic cations**

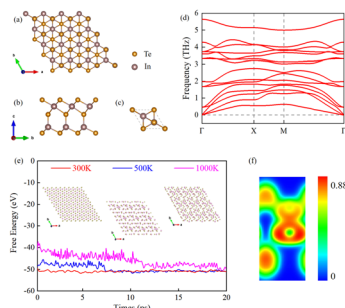
Dejan B. Milošević\* and Dino Habibović





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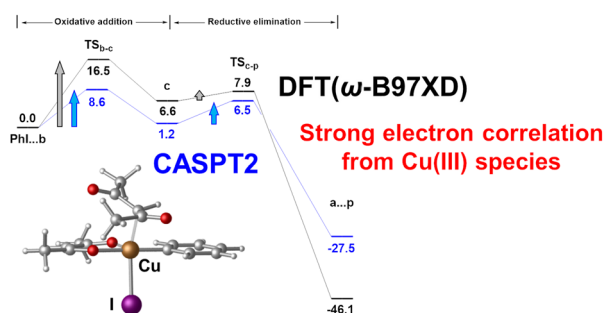
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### Electron transport, ferroelectric, piezoelectric and optical properties of two-dimensional $\text{In}_2\text{Te}_3$ : a first-principles study

Yuanmao Pu, Yumin Li, Zhibin Qiu, Lang Zhou, Chuanli Fang, Yaya Lou, Bing Lv, Jun Wei, Wenzhong Wang and Qingping Dai\*

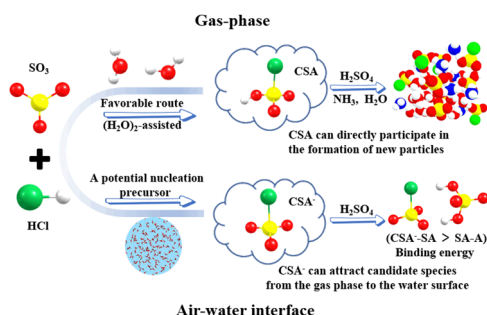
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### How does multi-reference computation change the catalysis chemistry? DFT and CASPT2 studies of the Cu-catalysed coupling reactions between aryl iodides and $\beta$ -diketones

Nan He, Naoki Nakatani\* and Masahiko Hada

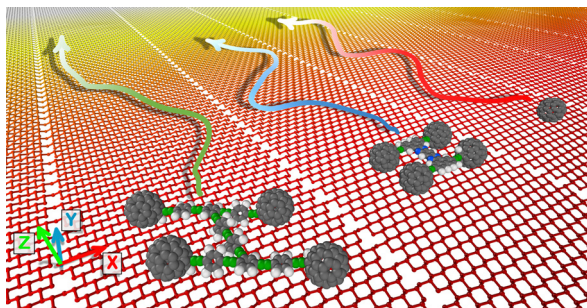
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### Significant influence of water molecules on the $\text{SO}_3 + \text{HCl}$ reaction in the gas phase and at the air–water interface

Yang Cheng, Chao Ding, Hui Wang, Tianlei Zhang,\* Rui Wang, Balaganesh Muthiah, Haitong Xu, Qiang Zhang and Min Jiang

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### Motion of nanovehicles on pristine and vacancy-defected silicene: implications for controlled surface motion

Mehrdad Youzi, Mohammad Kianezhad, Mehran Vaezi and Hossein Nejat Pishkenari\*

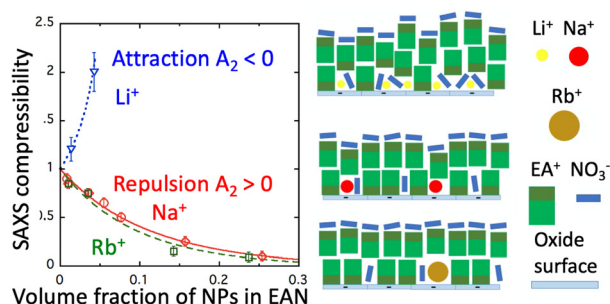


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# Ion specific tuning of nanoparticle dispersion in an ionic liquid: a structural, thermoelectric and thermo-diffusive investigation

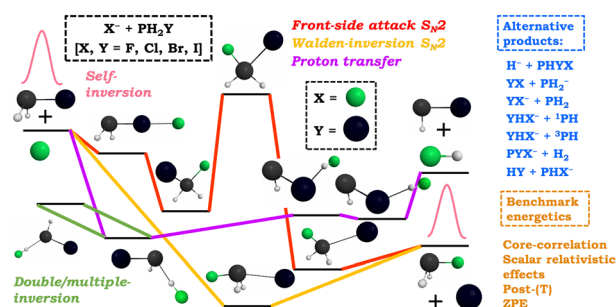
T. Fiuza, M. Sarkar, J. C. Riedl, M. Beaughon, B. E. Torres Bautista, K. Bhattacharya, F. Cousin, E. Barruet, G. Demouchy, J. Depeyrot, E. Dubois, F. Gélébart, V. Geertsens, G. Mériguet, L. Michot, S. Nakamae, R. Perzynski\* and V. Peyre



28925

# Phosphorus-centered ion–molecule reactions: benchmark *ab initio* characterization of the potential energy surfaces of the $X^- + PH_2Y$ [ $X, Y = F, Cl, Br, I$ ] systems

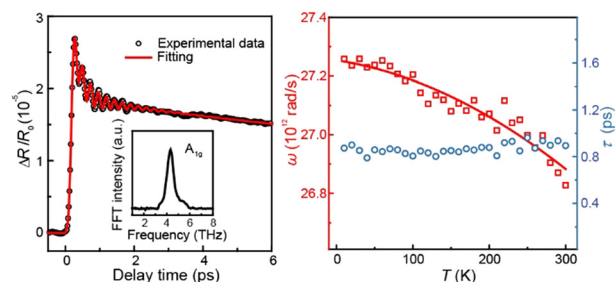
Boldizsár Ballay, Tímea Szűcs, Dóra Papp\* and Gábor Czakó\*



28941

# Resonance-enhanced excitation and relaxation dynamics of coherent phonons in Fe<sub>1.14</sub>Te

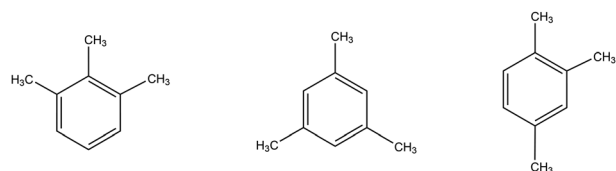
Ning Li, Chenhui Zhang, Weizheng Liang, Yaohua Jiang, Xi-Xiang Zhang, Yang Mi\* and Sheng-Nian Luo



28948

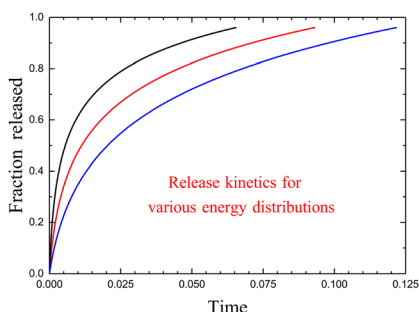
# A kinetic study of the reactions of atomic bromine with the trimethylbenzenes

John M. Roscoe



## RESEARCH PAPERS

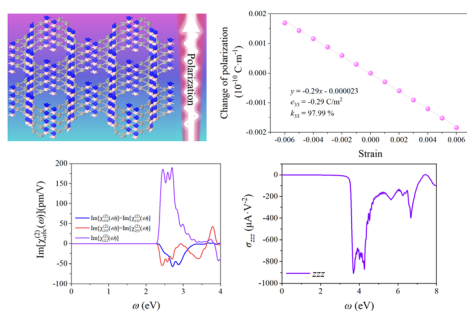
28955



## Release of molecules from nanocarriers

Vladimir P. Zhdanov

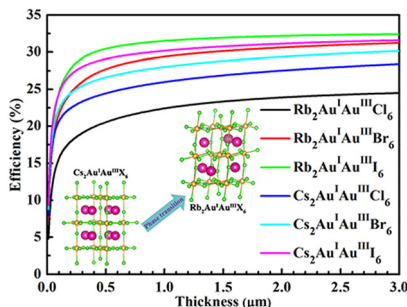
28965



## Three-dimensional porous borocarbonitride composed of pentagonal motifs as a high-performance pyroelectric material

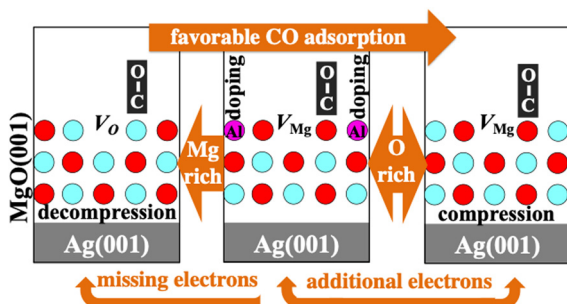
Changsheng Hou, Yiheng Shen, Jiaqi Xin, Yaguang Guo\* and Qian Wang\*

28974

A theoretical exploration of the structural feature, mechanical, and optoelectronic properties of Au-based halide perovskites  $A_2Au^I Au^{III}X_6$  ( $A = Rb, Cs; X = Cl, Br, I$ )

Diwen Liu,\* Huihui Zeng, Huan Peng and Rongjian Sa\*

28982



## CO adsorption on MgO thin-films: formation and interaction of surface charged defects

Raphael da Silva Alvim,\* Itamar Borges Jr., Rita Maria Brito Alves, Rodrigo B. Capaz and Alexandre Amaral Leitão

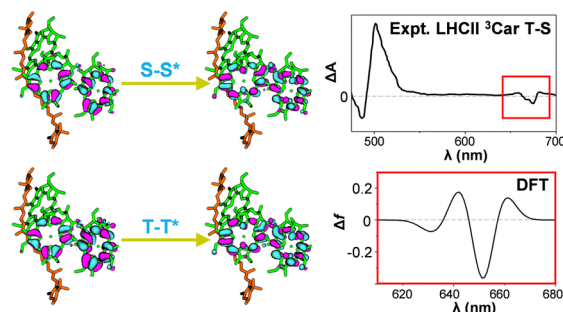


## RESEARCH PAPERS

28998

# Unraveling the electronic origin of a special feature in the triplet-minus-singlet spectra of carotenoids in natural photosystems

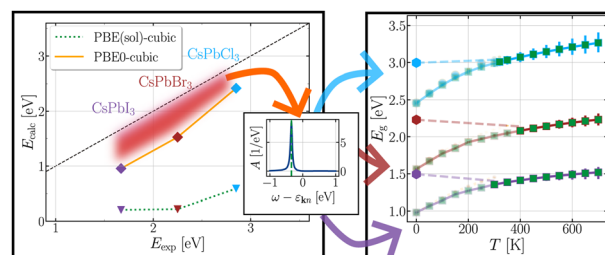
Agostino Migliore,\* Stefano Corni, Alessandro Agostini and Donatella Carbonera\*



29017

# Ab-initio calculations of temperature dependent electronic structures of inorganic halide perovskite materials

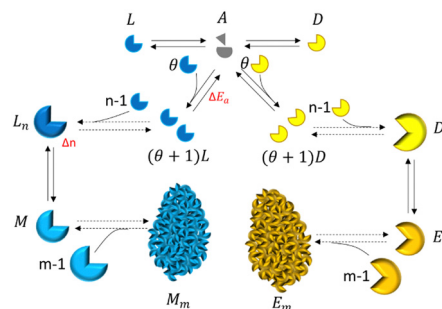
Milan Jocić and Nenad Vukmirović\*



29032

# Variations in activation energy and nuclei size during nucleation explain chiral symmetry breaking

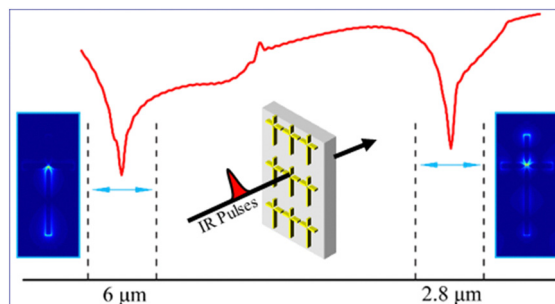
A. Arango-Restrepo,\* D. Barragán and J. M. Rubi

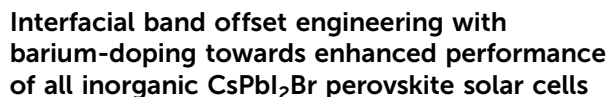


29042

# A super asymmetric cross antenna structure with tunable dual-frequency resonances

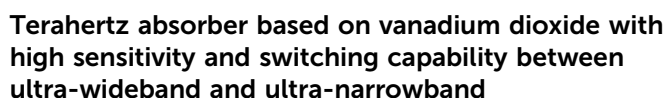
Haiyan Xu and Jianping Wang\*





Sachin R. Rondiya,\* Sawanta S. Mali,\* Anurag Roy,  
Gajendra Kumar Inwati, Ganesh K. Rahane,  
Yogesh A. Jadhav, Sunil Suresh, Tushar Debnath,  
Chang Kook Hong and Nelson Y. Dzade\*

29061



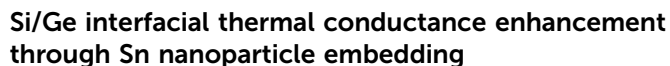
Qianli Song, Xingxin Cheng, Tao Liu, Yanyu Zhang,  
Zigang Zhou,\* Yongjia Yang,\* Hao Chen, Bin Tang,  
Jing Chen and Zao Yi\*

29070



Jerry Kamer, Domenik Schleier, Merel Donker,  
Patrick Hemberger, Andras Bodi and Jordy Bouwman\*

29080



Ying-Guang Liu,\* Heng-Xuan Li, Yu-Jun Qiu, Xin Li and  
Chun-Pu Huang

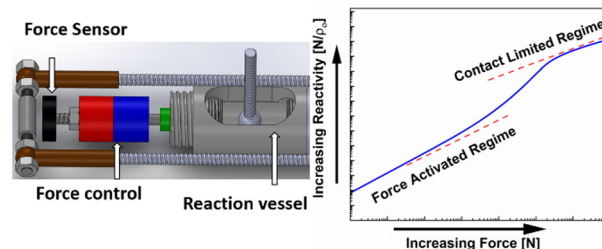


## RESEARCH PAPERS

29088

**Mechanistic model for quantifying the effect of impact force on mechanochemical reactivity**

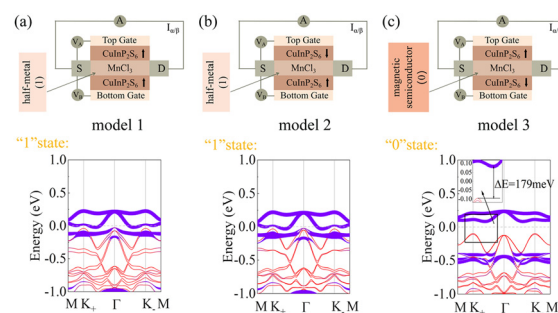
Emmanuel Nwoye, Shivanjan Raghuraman, Maya Costales, James Batteas and Jonathan R. Felts\*



29098

**Nonvolatile magnetoelectric coupling in two-dimensional van der Waals sandwich heterostructure  $\text{CuInP}_2\text{S}_6/\text{MnCl}_3/\text{CuInP}_2\text{S}_6$** 

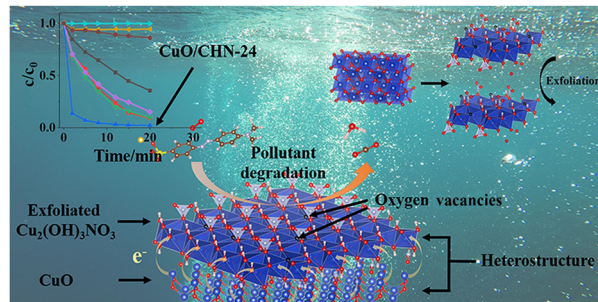
Zichun Wang, Honggang Pan\* and Baozeng Zhou\*



29108

**Plasma synthesis of oxygen vacancy-rich  $\text{CuO}/\text{Cu}_2(\text{OH})_3\text{NO}_3$  heterostructure nanosheets for boosting degradation performance**

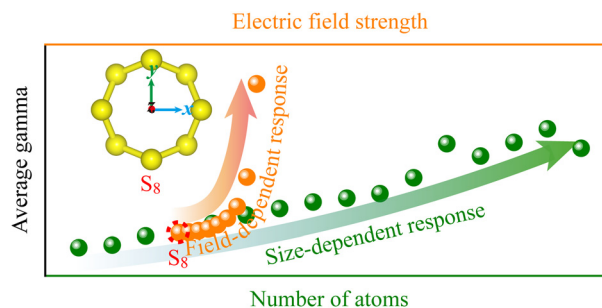
Zikun Yang, Xiangfeng Peng, Jingxuan Zheng and Zhao Wang\*



29120

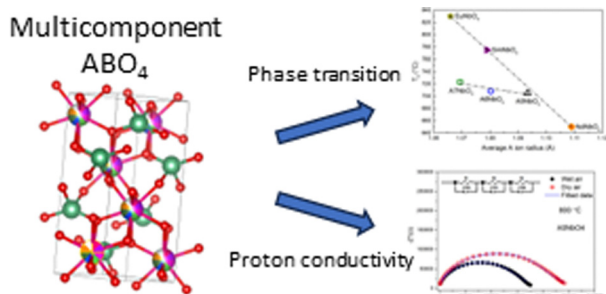
**Lone-pair, electron-dominated, nonlinear optical responses in sulfur clusters and electric tunability properties**

Quanjie Zhong\*



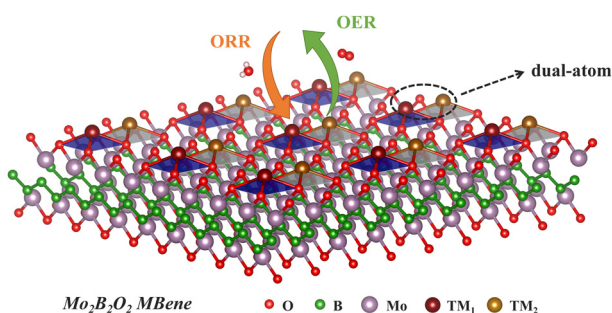
## RESEARCH PAPERS

29127

Proton conductivity in multi-component ABO<sub>4</sub>-type oxides

Ashraf A.A. Elameen, Arkadiusz Dawczak, Tadeusz Miruszewski, Maria Gazda and Sebastian Wachowski\*

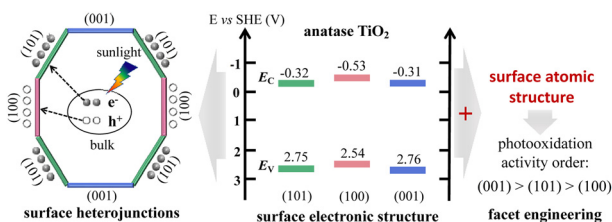
29135



## Rational design of 2D MBene-based bifunctional OER/ORR dual-metal atom catalysts: a DFT study

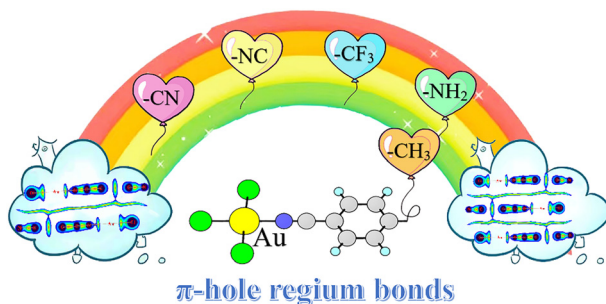
Yiwei Mou, Yanwei Wang, Jin Wan, Guangxu Yao, Chuanzhen Feng, Huijuan Zhang and Yu Wang\*

29143

Water effect on the band edges of anatase TiO<sub>2</sub> surfaces: A theoretical study on charge migration across surface heterojunctions and facet-dependent photoactivity

Jie-Qiong Li,\* Jin-Yuan Hu and Jun Cheng\*

29155

Gold(III) derivatives as the noncovalent interaction donors: theoretical study of the  $\pi$ -hole region bonds

Jiajing Yan, Yanli Zeng, Lingpeng Meng, Xiaoyan Li\* and Xueying Zhang\*

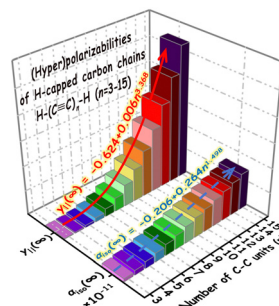


## RESEARCH PAPERS

29165

### Size dependence of optical nonlinearity for H-capped carbon chains, $\text{H}-(\text{C}\equiv\text{C})_n-\text{H}$ ( $n = 3-15$ ): analysis of its nature and prediction for long chains

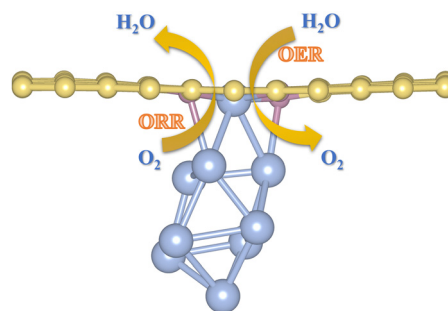
Zeyu Liu,\* Jiaojiao Wang, Qing Zhou, Tian Lu,\* Xia Wang, Xiufen Yan, Mengdi Zhao and Aihua Yuan\*



29173

### Construction of highly active $\text{FeN}_4\text{@Fe}_x(\text{OH})_y$ cluster composite sites for the oxygen reduction reaction and the oxygen evolution reaction

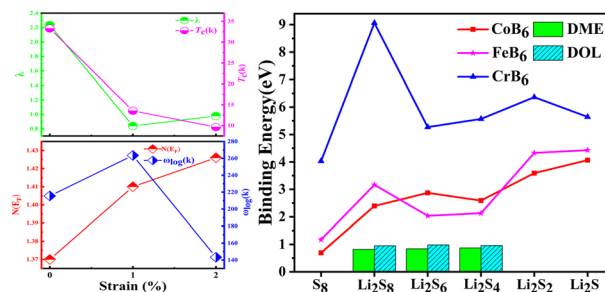
Yulin Zhang, Xihao Chen, Siyu Gan, Yu Hu, Yi Tian, Shiyu Wang, Long Chen, Junping Xiao\* and Ning Wang\*



29182

### Theoretical study on the superconductivity of graphene-like $\text{TMB}_6$ ( $\text{TM} = \text{Cr}, \text{Fe}$ and $\text{Co}$ ) monolayer and its potential anchoring and catalytic properties for lithium-sulfur batteries

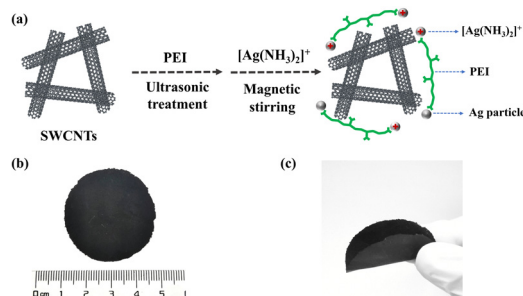
Siqi Liu, Rongfang Huang, Jianhua Hou\* and Qian Duan



29192

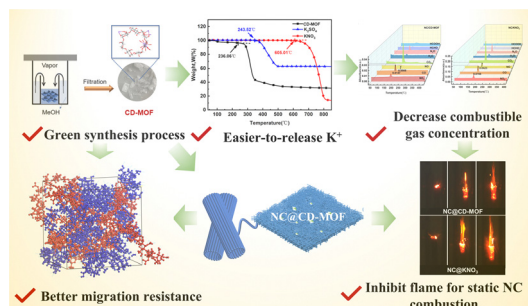
### N-type silver ammonia-polyethyleneimine/single-walled carbon nanotube composite films with enhanced thermoelectric properties

Zan Li, Duo Jiang, Jiayan Gong, Yi Li, Ping Fu, Yunfei Zhang\* and Feipeng Du\*



## RESEARCH PAPERS

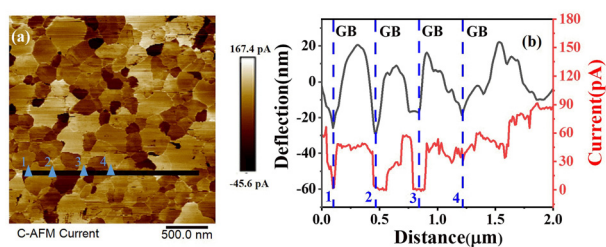
29201



### Enhancing propellant performance through intermolecular interactions: cyclodextrin-based MOF loading in nitrocellulose

Wenjia Li, Yuanqi Gan, Yu Li, Shiyong Li, Jinghao Liang, Wenhao Fan, Zichun Yu, Yichang Li, Yajun Ding,\* Zhongliang Xiao and Jie Zhou\*

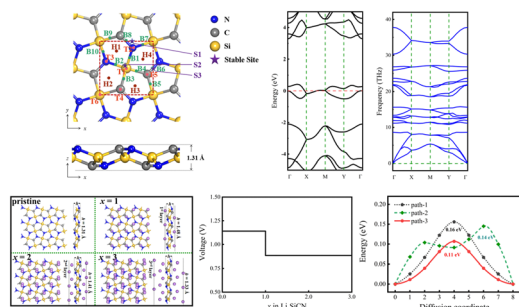
29211



### The synergistic effect of trap deactivation and hysteresis suppression at grain boundaries in perovskite interfaces *via* multifunctional groups

Fei Wang, Xiaohu Ma, Wei Huang, Jun Han, Dandan Luo, Chong Jia and Yiqing Chen\*

29224

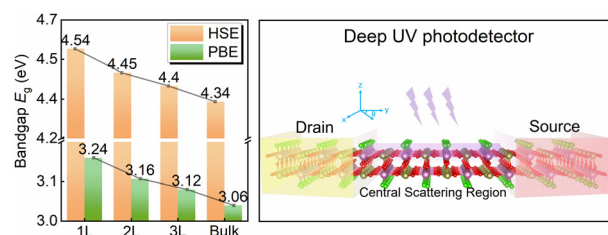


## RESEARCH PAPERS

29241

## Two-dimensional $\text{InTeClO}_3$ : an ultrawide-bandgap material with potential application in a deep ultraviolet photodetector

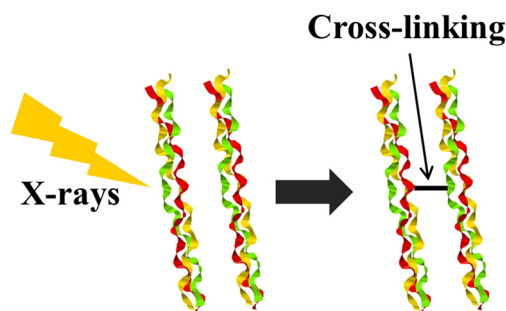
Meiyang Yu, Fumin Zhang, Wenjiang Gao, Huimin Shen, Lili Kang,\* Lin Ju\* and Huabing Yin\*



29249

## Ionizing radiation induces cross-linking of two noncovalently bound collagen mimetic peptide triple helices in the absence of a molecular environment

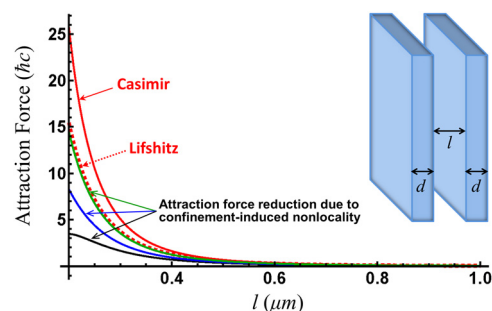
Marwa Abdelmouleh, Muhamed Amin, Mathieu Lalande, Thomas Schlathöller and Jean-Christophe Pouilly\*



29257

## Confinement-induced nonlocality and casimir force in transdimensional systems

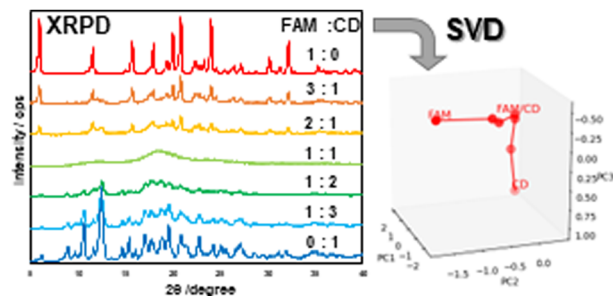
Igor V. Bondarev,\* Michael D. Pugh, Pablo Rodriguez-Lopez, Lilia M. Woods and Mauro Antezza



29266

## Using singular value decomposition to analyze drug/ $\beta$ -cyclodextrin mixtures: insights from X-ray powder diffraction patterns

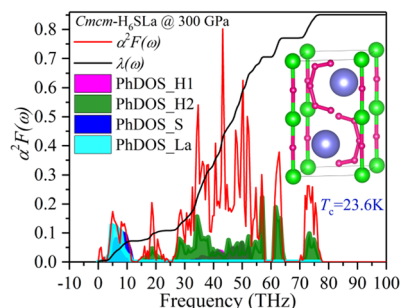
Kanji Hasegawa, Satoru Goto,\* Chihiro Tsunoda, Chihiro Kuroda, Yuta Okumura, Ryosuke Hiroshige, Ayako Wada-Hirai, Shota Shimizu, Hideshi Yokoyama and Tomohiro Tsuchida





## RESEARCH PAPERS

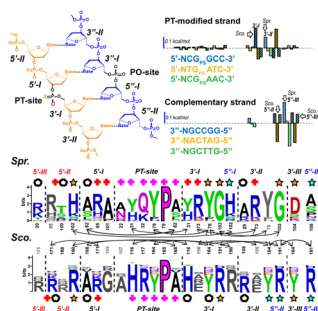
29283



### First-principles study of the structures and superconductivity of H–S–La systems under high pressure

Yin L. Xu, Yang M. Chen,\* Xiao Z. Yan,\* Yi B. Huang, Xing Z. Zhou, Quan X. Wu, Xiao W. Sheng and Fang G. Kuang

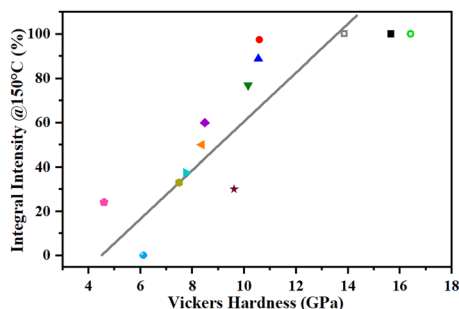
29289



### Understanding base and backbone contributions of phosphorothioate DNA for molecular recognition with SBD proteins

Jiayi Li, Shenggan Luo, Xingyu Ouyang, Geng Wu, Zixin Deng, Xinyi He and Yi-Lei Zhao\*

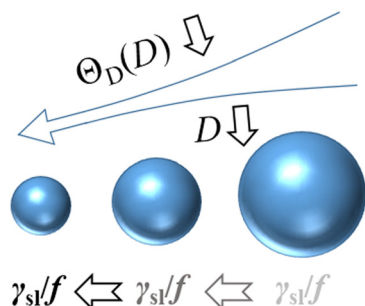
29303



### Quantifying rigidity for thermally stable Cr<sup>3+</sup> phosphors

Shaojian Xu, Jiahao Feng, Daidi Zhang, Biqian Zhang, Dawei Wen,\* Mingmei Wu\* and Junhao Li

29310



### Size effect on Debye temperature of metal crystals

Xiaobao Jiang,\* Hongchao Sheng and Beibei Xiao

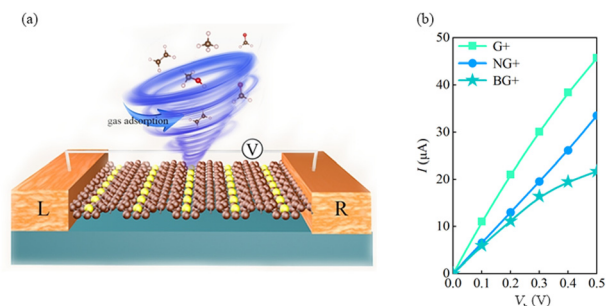


## RESEARCH PAPERS

29315

# Design and analysis of a 2D grapheneplus (G<sup>+</sup>)-based gas sensor for the detection of multiple organic gases

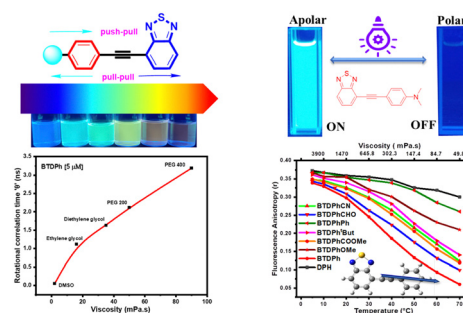
Danfeng Qin, Tong Chen,\* Luzhen Xie, Ning Yang, Cheng Luo and Guanghui Zhou



29327

# Effects of donor and acceptor substituents on the photophysics of 4-ethynyl-2,1,3-benzothiadiazole derivatives

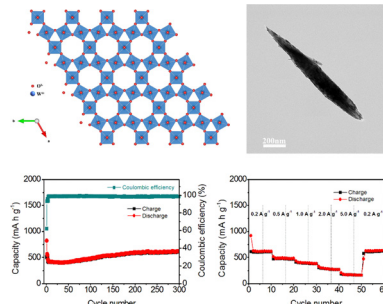
Asit Kumar Pradhan, Manaswini Ray, Venkatakrishnan Parthasarathy\* and Ashok Kumar Mishra\*



29341

# One-step construction of hexagonal WO<sub>3</sub> nano-shuttles with enhanced lithium storage performance

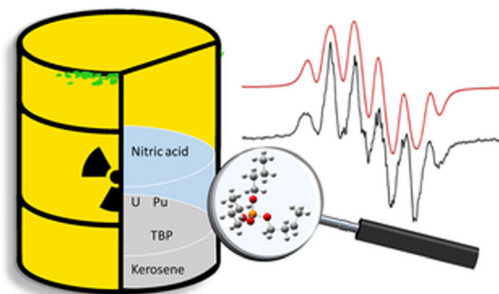
Fangyuan Dong, Xuelu Dong, Chonggang Fu,\* Shuo Tao, Haibo Li, Suyuan Zeng\* and Lei Wang\*



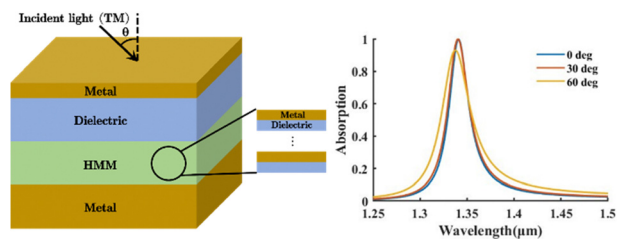
29350

# Radicals from tributyl phosphate decomposition: a combined electron paramagnetic resonance spectroscopic and computational chemistry investigation

Ilya S. Sosulin, Delaney H. Ryan and Aliaksandra Lisouskaya\*



29358



### A tunable wide-angle narrowband perfect absorber based on an optical cavity containing hyperbolic metamaterials

Zhenlong Xie, Xu Zhu, Yijing Deng and Yihang Chen\*

