

## IN THIS ISSUE

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## EDITORIAL

15081

### Stability and properties of new-generation metal and metal-oxide clusters down to subnanometer scale

MariLa Pilar de Lara-Castells,\* Cristina Puzzarini,\* Vlasta Bonačić-Koutecký,\* M. Arturo López-Quintela\* and Stefan Vajda\*

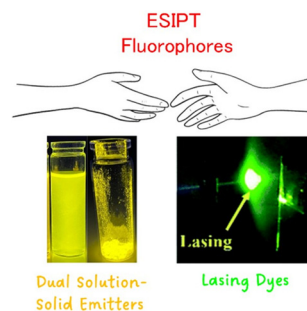


## REVIEW

15085

### Solid-state emitters presenting a modular excited-state proton transfer (ESIPT) process: recent advances in dual-state emission and lasing applications

Martyna Durko-Maciag, Gilles Ulrich, Denis Jacquemin, Jaroslaw Mysliwiec\* and Julien Massue\*



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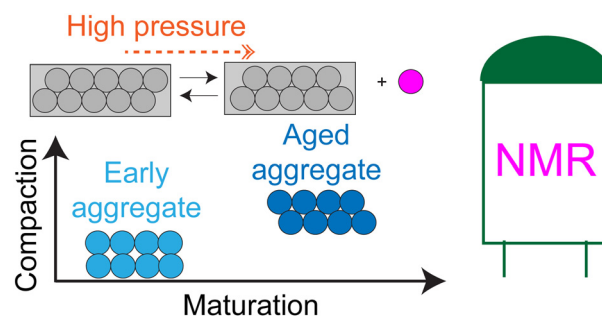


## COMMUNICATIONS

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**Maturation of amyloid  $\beta$  fibrils alters their molecular stability**

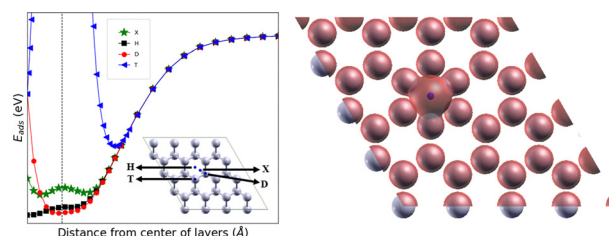
Stefan Becker, Karin Giller, Daniel Sieme and Nasrollah Rezaei-Ghaleh\*



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**Hydrogen adsorption and diffusion through a two dimensional sheet of lithium: a first principles study**

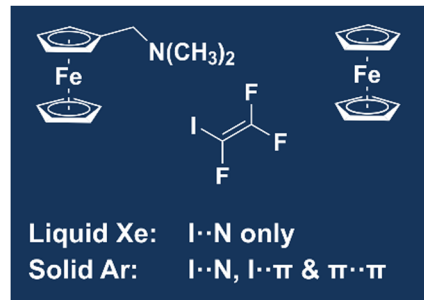
Shrijan Roy, Prince Singh, Kiran Yadav and Nirat Ray\*



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**Simultaneous observation of halogen–lone pair and halogen– $\pi$  interactions of ferrocene derivatives under cryogenic conditions**

Nora M. Kreienborg, Felix Otte, Carsten Strohmann and Christian Merten\*

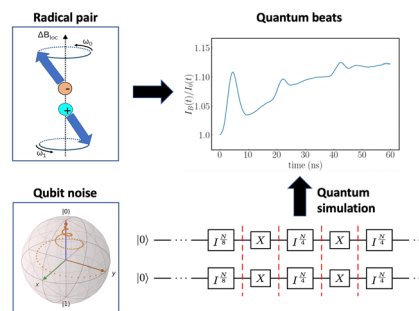


## RESEARCH PAPERS

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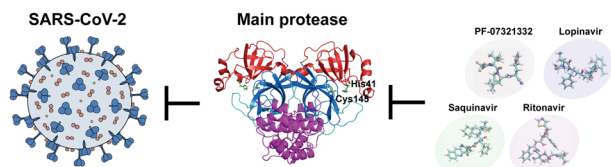
**Hamiltonian simulation of quantum beats in radical pairs undergoing thermal relaxation on near-term quantum computers**

Meltem Tolunay, Ieva Liepuoniute, Mariya Vyushkova and Barbara A. Jones\*



## RESEARCH PAPERS

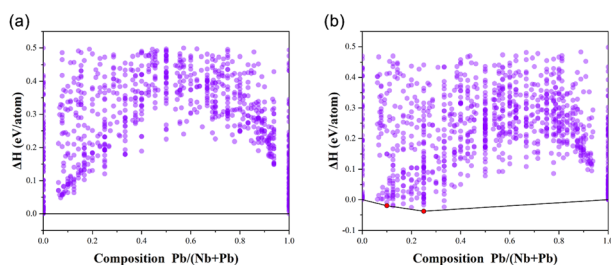
15135



### Binding kinetics study of SARS-CoV-2 main protease and potential inhibitors *via* molecular dynamics simulations

Xingyu Li, Zhou Fang, Dechang Li\* and Zhenhai Li\*

15146



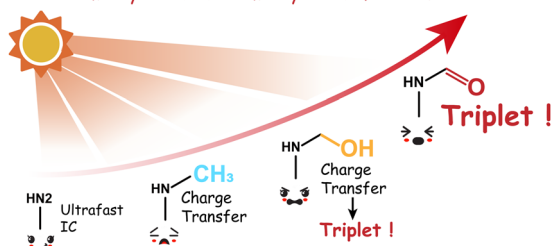
### Scanning the latent phases and superconductivity in the Nb–Pb system at high pressure

Yanqing Qin, Jiexi Song, Xinyu Chen, Diwei Shi,\* Rongrong Ren, Yaocen Wang, Xiaojun Bai, Xiaoguang Yang\* and Chongde Cao\*

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### Potential Damage is Escalating!

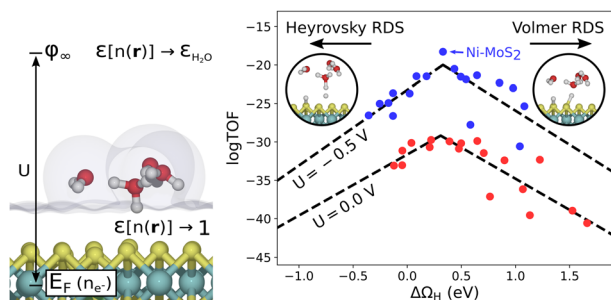
methylation and demethylation of Ado RNA



### Distinct doorway states lead to triplet excited state generation in epigenetic RNA nucleosides

Danhong Wang, Xueli Wang,\* Peipei Jin, Yusong Zhou, Menghui Jia, Haifeng Pan, Zhenrong Sun and Jinquan Chen\*

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### Is the doped MoS<sub>2</sub> basal plane an efficient hydrogen evolution catalyst? Calculations of voltage-dependent activation energy

Sander Ø. Hanslin, Hannes Jónsson and Jaakko Akola\*

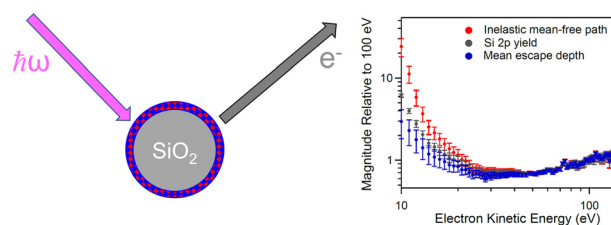


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### Inelastic mean-free path and mean escape depth of 10–140 eV electrons in SiO<sub>2</sub> nanoparticles determined by Si 2p photoelectron yields

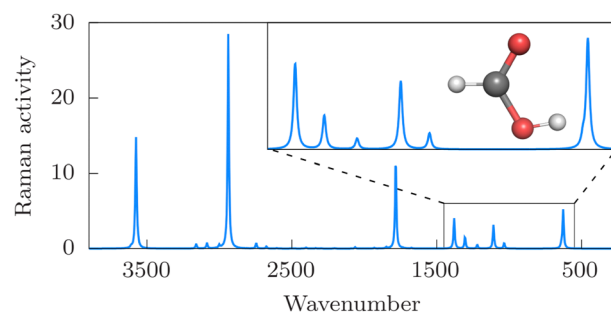
E. Antonsson, F. Gerke, B. Langer, C. Goroncy, T. Dresch, T. Leisner, C. Graf and E. Rühl\*



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### Vibrational infrared and Raman spectra of HCOOH from variational computations

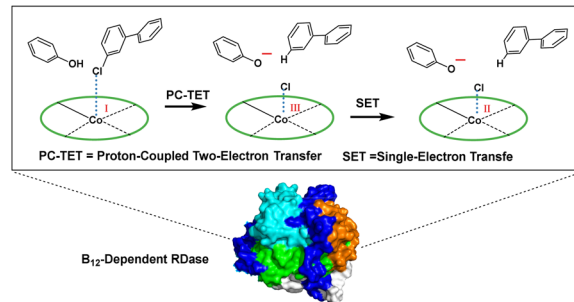
Gustavo Avila, Alberto Martin Santa Daria and Edit Mátyus\*



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### Mechanistic insight into the *Dehalococcoides*-mediated reductive dechlorination of polychlorinated biphenyls

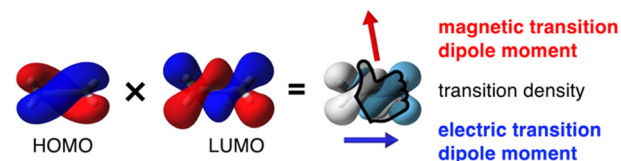
Shangwei Zhang,\* Wei Ouyang, Xinghui Xia, Wu Wen,\* Lorenz Adrian and Gerrit Schüürmann



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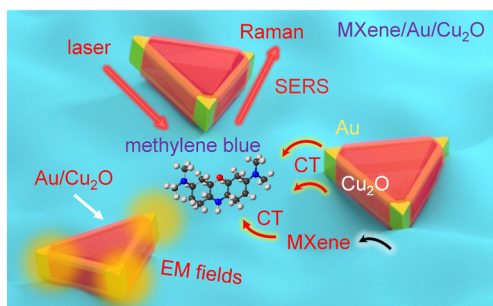
### The fundamental relation between electrohelicity and molecular optical activity

Marc H. Garner\* and Clemence Corminboeuf



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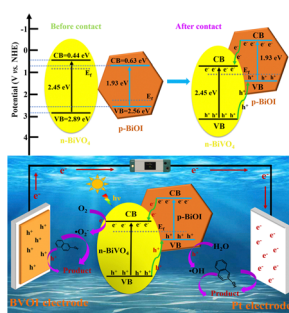
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### Optimized electromagnetic enhancement and charge transfer in MXene/Au/Cu<sub>2</sub>O hybrids for achieving efficient SERS

Yi-Xin Zhao, Zi-Xing Zheng, Liu-Shuai Zhang, Jing-Ru Feng, Liang Ma\* and Si-Jing Ding\*

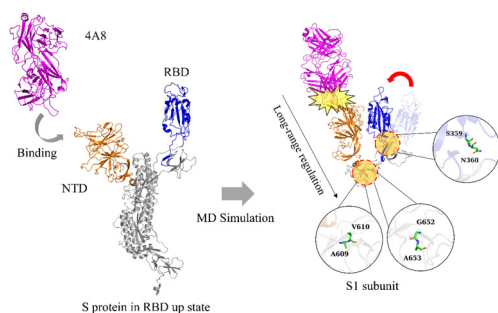
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### Construction of a type-II BiVO<sub>4</sub>/BiOI heterojunction for efficient photoelectrocatalytic degradation of $\beta$ -naphthol and coal gasification wastewater under visible-light irradiation

Haiyang Fan, Guiyun Yi,\* Zhengting Zhang, Yanan Zhao, Qinglin Hou, Chuanxiang Zhang,\* Lunjian Chen, Yulong Zhang and Qi Sun

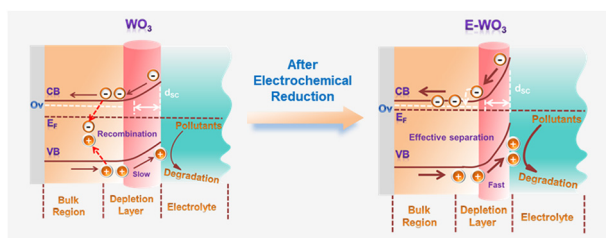
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### Molecular mechanism study of the structural regulation of the N-terminal domain binding antibody on the receptor binding domain of SARS-CoV-2

Hongtao Liu, Zihui Tian, Shuai Yuan\* and Shuangyan Zhou\*

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### Improved photoelectrocatalytic performances over electrochemically reduced WO<sub>3</sub>: implications of oxygen vacancies

Yunni Liu, Wang Yao and Jun Lin\*

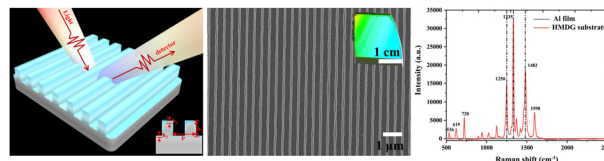


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## Hybrid metal-dielectric gratings (HMDGs) as an alternative UV-SERS substrate

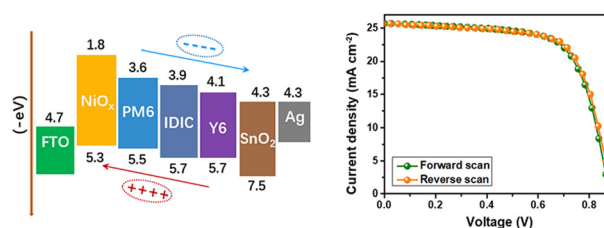
Jie Zheng,\* Xianchao Liu, Mingyang Tian, Yarong Su and Ling Li\*



15263

## Improving the performance of ternary organic solar cells using metal oxides as charge-transport layers

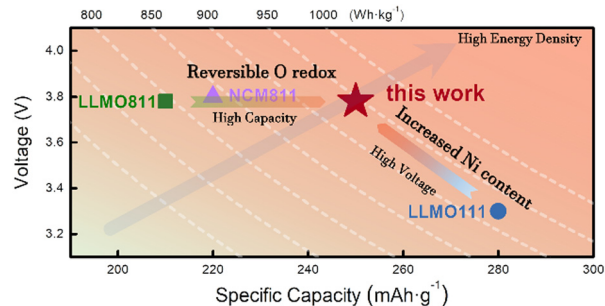
Zhihai Liu, Lei Wang, Xiaoyin Xie\* and Ping Chen\*



15271

## Highly activated oxygen redox enabling large-capacity Li-rich layered manganese-based oxide cathodes

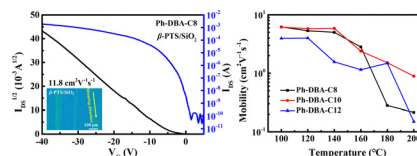
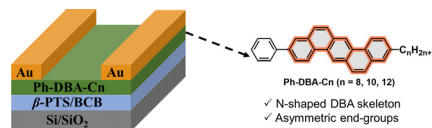
Feng Lin, Junhao Wen, Huali Zhu, Yu Tang, Zihua Li, Tao Li, Yanxia Wang\* and Zhaoyong Chen\*



15279

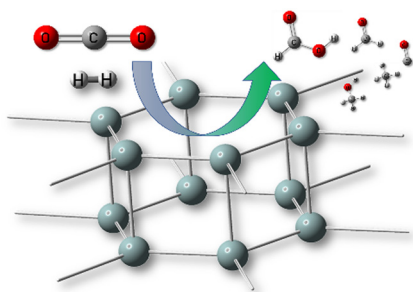
Asymmetric liquid crystalline dibenzo[*a,h*]anthracenes for organic semiconductors with high mobility and thermal stability

Yucong Bao, Liang Zhang, Haoming Wei, Bingqiang Cao\* and Tengzhou Yang\*



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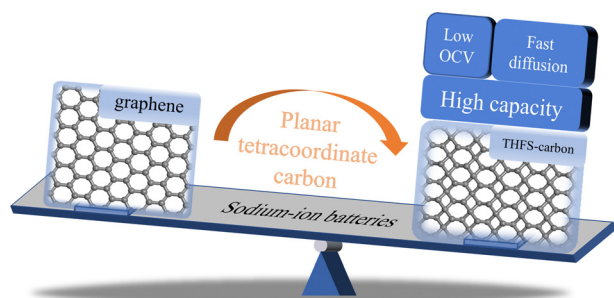
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### Catalytic activity of silicene bilayers for CO<sub>2</sub> reduction: a theoretical approach

Wilmer E. Vallejo Narváez,\*  
Cesar Gabriel Vera de la Garza and  
Serguei Fomine\*

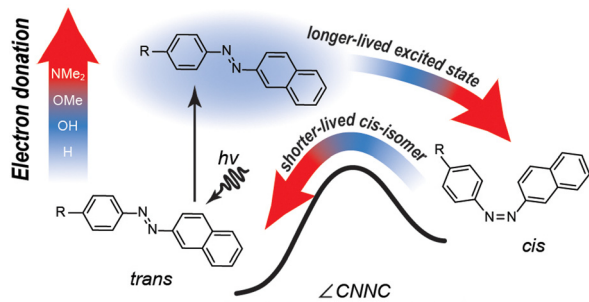
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### THFS-carbon: a theoretical prediction of metallic carbon allotrope with half-auxeticity, planar tetracoordinate carbon, and potential application as anode for sodium-ion batteries

Tian-Kai Li, Xiao-Juan Ye, Lan Meng and  
Chun-Sheng Liu\*

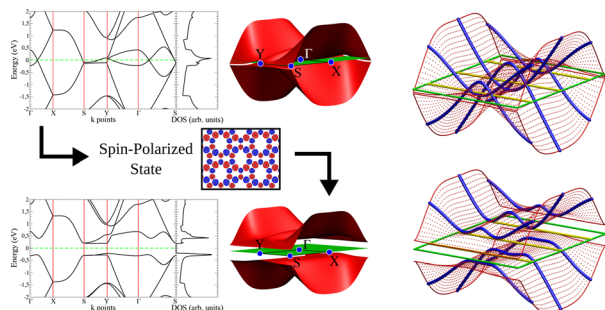
15302



### Ultra-fast excited-state dynamics of substituted *trans*-naphthalene azo moieties

Robert C. Hamburger, Tao Huang, Shea M. Martin,  
Craig A. Pointer, Lisa A. Fredin\* and Elizabeth R. Young\*

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### Spin-polarized electronic properties of naphthylene-based carbon nanostructures

Mário Rocha dos Santos, Mayada Fadel,  
Paloma Vieira Silva, Vincent Meunier and  
Eduardo Costa Girão\*



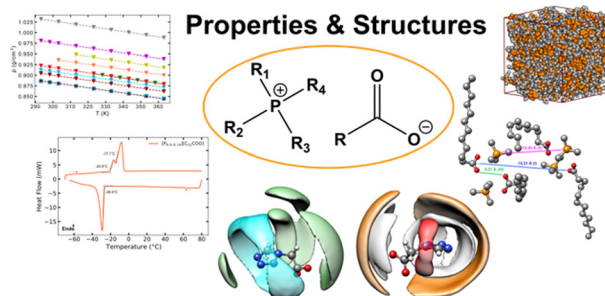


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## Alkylphosphonium carboxylate ionic liquids with tuned microscopic structures and properties

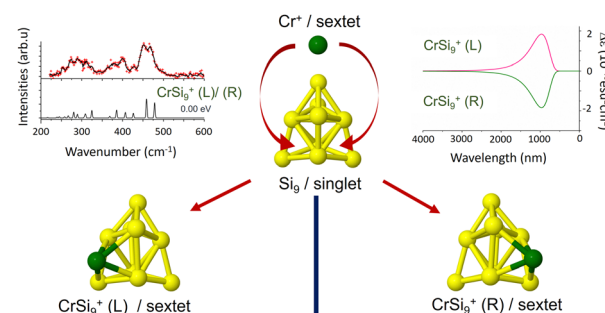
N. Scaglione, J. Avila, E. Bakis, A. Padua\* and M. Costa Gomes\*



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Small chromium-doped silicon clusters  $\text{CrSi}_n$ : structures, IR spectra, charge effect, magnetism and chirality

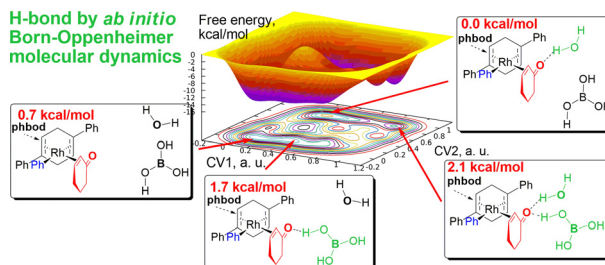
Bao-Ngan Nguyen-Ha, Ngoc Thach Pham, Pieterjan Claes, Peter Lievens, André Fielicke, Vu Thi Ngan, Minh Tho Nguyen\* and Ewald Janssens\*



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Realistic modelling of hydrogen bonding of 2-cyclohexenone with  $\text{H}_2\text{O}$  and  $\text{H}_3\text{BO}_3$  in the outer coordination sphere of a chiral diene/Rh(I) complex by *ab initio* molecular dynamics

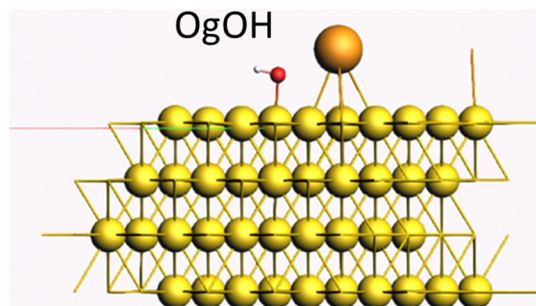
Eric Assen B. Kantchev\* and Petko S. Petkov\*



15362

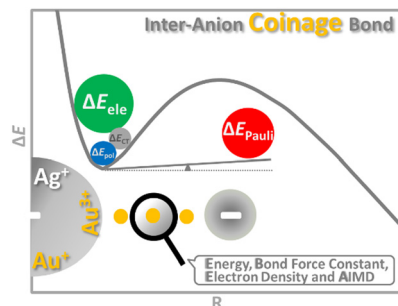
## A theoretical study of the adsorption behavior of superheavy 7p-elements and their compounds on a surface of gold in comparison with their lighter homologs

Anton Ryzhkov, Valeria Pershina, Miroslav Iliaš\* and V. Shabaev



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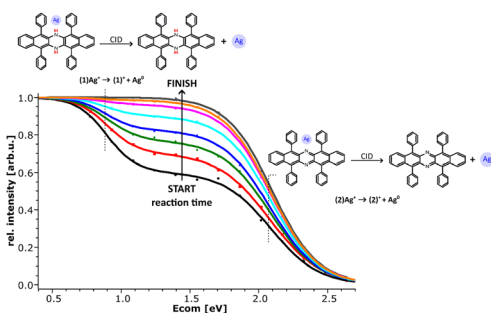
15371



## On the nature of inter-anion coinage bonds

Jiayao Li, Qiuyan Feng, Changwei Wang\* and Yirong Mo\*

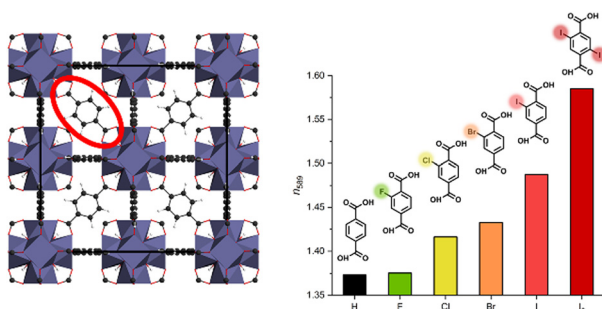
15382



## Silver cation tagged on 5,7,12,14-tetraphenyl-6,13-diazapentacene and its dihydro-form

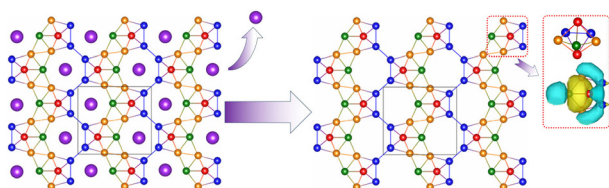
Marina Kinzelmann, Johannes Oswald, Holger Elsen, Vera Warmbrunn, Miriam Hauschild, Sjoerd Harder, Milan Kivala and Thomas Drewello\*

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Development of high refractive index UiO-66 framework derivatives *via* ligand halogenation

Marvin Treger, Adrian Hannebauer, Peter Behrens and Andreas M. Schneider\*

15400



## Superconducting boron allotrope featuring pentagonal bipyramid at ambient pressure

Shuai Han, Yunxian Liu,\* Chao Wang, Wencai Yi, Xin Chen, Yongsheng Zhang and Xiaobing Liu\*

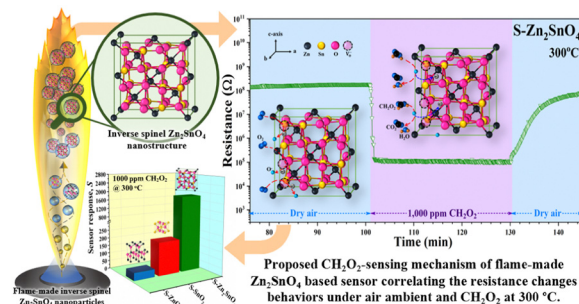


## RESEARCH PAPERS

15407

### Comparative study on formic acid sensing properties of flame-made $\text{Zn}_2\text{SnO}_4$ nanoparticles and its parent metal oxides

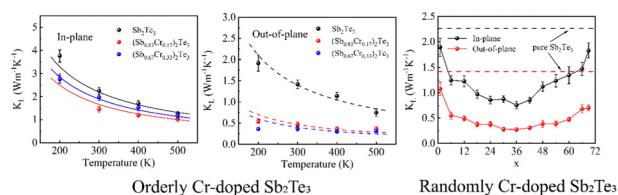
Matawee Punginsang, Kanittha Inyawilert, Mameaseng Siriwalai, Anurat Wisitsoraat, Adisorn Tuantranont and Chaikarn Liewhiran\*



15422

### Tuning the lattice thermal conductivity of $\text{Sb}_2\text{Te}_3$ by Cr doping: a deep potential molecular dynamics study

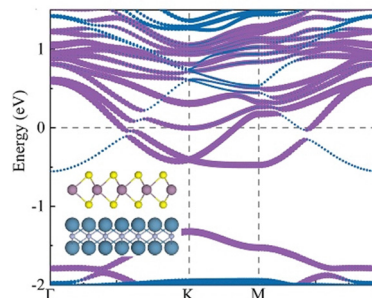
Pan Zhang, Wenkai Liao, Ziyang Zhu, Mi Qin, Zhenhua Zhang, Dan Jin, Yong Liu, Ziyu Wang, Zhihong Lu\* and Rui Xiong\*



15433

### Ohmic contacts of the two-dimensional $\text{Ca}_2\text{N}/\text{MoS}_2$ donor–acceptor heterostructure

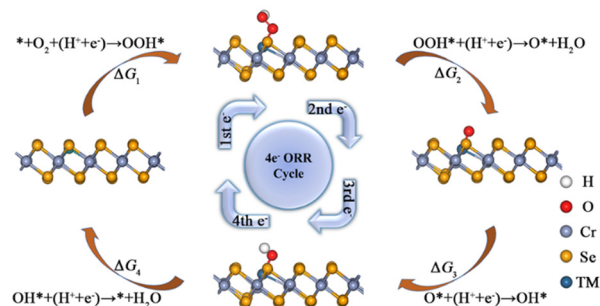
Xinxin Wang, Shiqiang Yu, Yushuo Xu, Baibiao Huang, Ying Dai\* and Wei Wei\*



15441

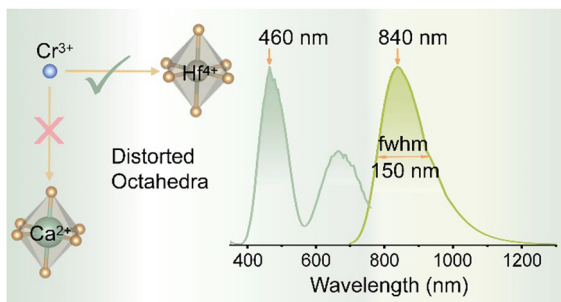
### First-principles study on the catalytic performance of transition metal atom-doped $\text{CrSe}_2$ for the oxygen reduction reaction

Long Lin, Yadan Sun, Kun Xie, Pei Shi, Xinyu Yang and Dongbin Wang\*



## RESEARCH PAPERS

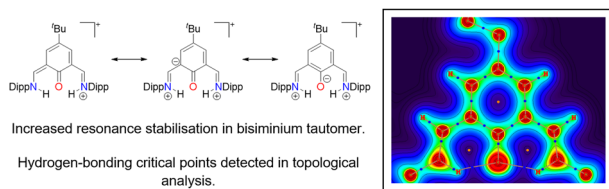
15452



### Understanding the broadband near-infrared luminescence in a highly distorted garnet Ca<sub>4</sub>HfGe<sub>3</sub>O<sub>12</sub>:Cr<sup>3+</sup> phosphor

Zurong Liao, Jiyou Zhong,\* Chaojie Li, Huan Jiang and Weiren Zhao\*

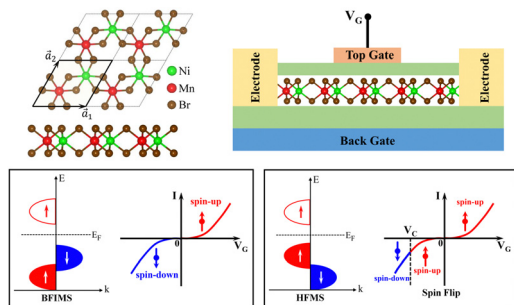
15463



### Hydrogen-bonding and resonance stabilisation effects in cationic bis(iminium) phenoxide diacids

Rebecca L. Jones, Louis J. Morris, Clement G. Collins Rice, Zoë R. Turner and Dermot O'Hare\*

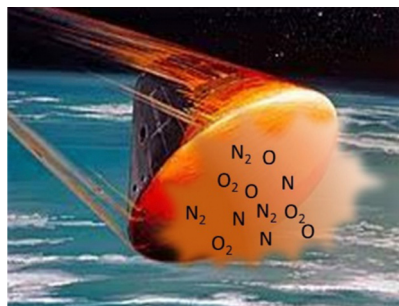
15469



### Bipolar ferrimagnetic semiconductor and doping concentration induced carrier spin flip in monolayer NiMnBr<sub>6</sub>

Chenchen Lou, Yujie Wang, Chunlan Ma and Jiayong Zhang\*

15479



### Informing air-carbon ablation modeling with theoretical calculations of atomic oxygen and nitrogen interacting with carbon surfaces

Reed Nieman, Michael Sands, Yingqi Wang, Timothy K. Minton, Erin E. Mussoni, Jeffrey Engerer and Hua Guo\*

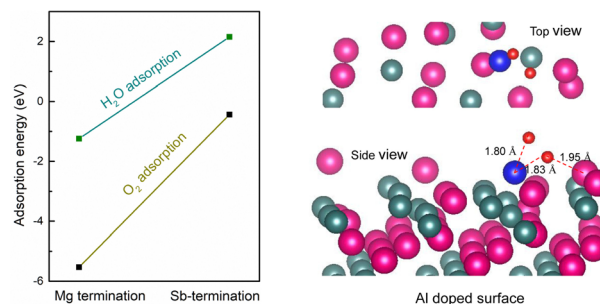


## RESEARCH PAPERS

15490

**First-principles study of O<sub>2</sub> and H<sub>2</sub>O adsorption on the Mg<sub>3</sub>Sb<sub>2</sub>(10–11) surface**

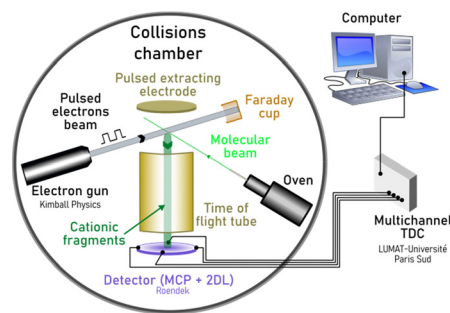
Juan Li, Kai Han, Bing Sun, Lianzhen Cao and Shuai Zhang\*



15497

**Electron-induced ionization and cationic fragmentations of the isolated molecule of 2,4-imidazolidinedione (hydantoin): a study of the relaxing path thresholds**

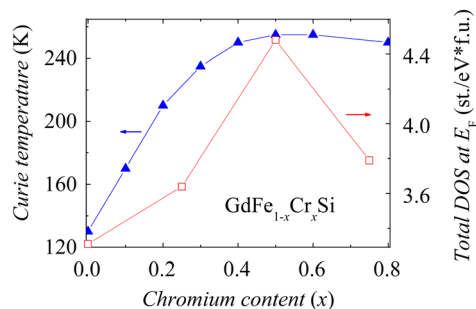
J.-P. Champeaux,\* P. Moretto-Capelle, J. Renoud, L. Polizzi, S. Faure, D. Castex, M. Gianesin, E. Panader, P. Paquier, W. Volondat, T. Salbaing, J. Riffaud, R. Point, P. Cafarelli and M. Sence



15508

**Magnetocaloric effect and magnetic ordering in GdFe<sub>1-x</sub>T<sub>x</sub>Si, T = Cr, V, Ni**

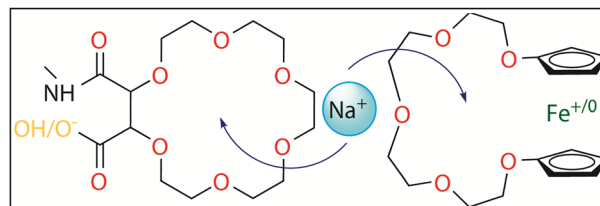
A. G. Kuchin,\* S. P. Platonov, R. D. Mukhachev, A. V. Lukoyanov, A. S. Volegov, V. S. Gaviko and M. Yu. Yakovleva



15518

**Cation recognition controlled by protonation or chemical reduction: a computational study**

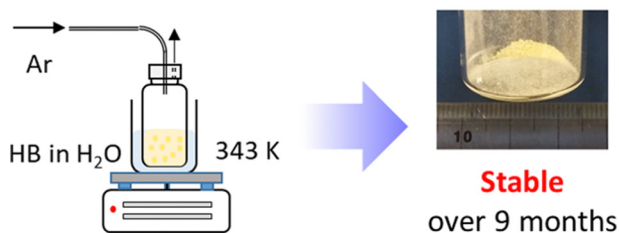
Renato Pereira Orenha,\* Alexandre Borges, Ana Livia de Oliveira Andrade, Sergio Eduardo Ferreira, Saulo Samuel Pereira Furtado, Vinicius Acir Glitz, Giovanni Finoto Caramori\* and Renato Luis Tame Parreira\*



## RESEARCH PAPERS

15531

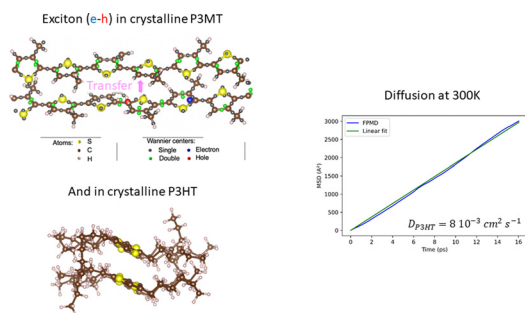
## Hydrogen boride (HB)



## Effective treatment of hydrogen boride sheets for long-term stabilization

Shin-ichi Ito, Miwa Hikichi, Natsumi Noguchi, Mei Yuan, Zihao Kang, Kosei Fukuda, Masahiro Miyauchi, Iwao Matsuda and Takahiro Kondo\*

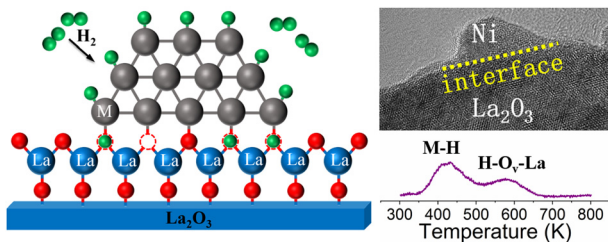
15539



## Exciton diffusion in poly(3-hexylthiophene) by first-principles molecular dynamics

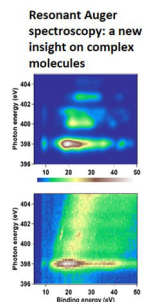
Chieck Oumar Diarra, Mauro Boero, Emilie Steveler, Thomas Heiser and Evelyne Martin\*

15547

Insights into the enhanced hydrogen adsorption on M/La<sub>2</sub>O<sub>3</sub> (M = Ni, Co, Fe)

Changyin Zhong, Yifei Yang,\* Yun Fang, Jun Chen, Bomin Feng, Hongbing Wang, Wenhua Luo and Yunxi Yao\*

15555



## Experimental and theoretical study of resonant core-hole spectroscopies of gas-phase free-base phthalocyanine

C. E. V. de Moura, J. Laurent, J. Bozek, M. Briant, P. Çarçal, D. Cubaynes, N. Shafizadeh, M. Simon, B. Soep, R. Püttner and G. Goldsztejn\*

