

## IN THIS ISSUE

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### Cover

See Olaf Brummel, Josef Mysliveček *et al.*, pp. 1630–1639. Image reproduced by permission of Josef Mysliveček from *Phys. Chem. Chem. Phys.*, 2024, 26, 1630.



### Inside cover

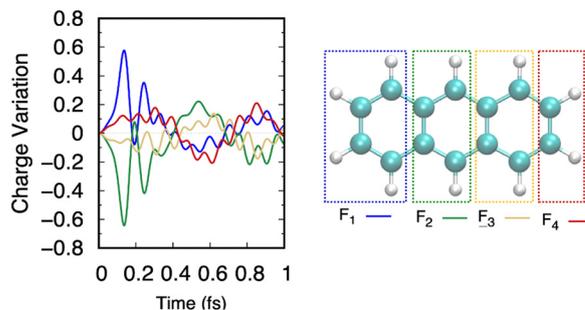
See Mathias Rapacioli *et al.*, pp. 1499–1515. Image reproduced by permission of Mathias Rapacioli and CNRS-5626 from *Phys. Chem. Chem. Phys.*, 2024, 26, 1499.

## REVIEWS

1499

### Addressing electronic and dynamical evolution of molecules and molecular clusters: DFTB simulations of energy relaxation in polycyclic aromatic hydrocarbons

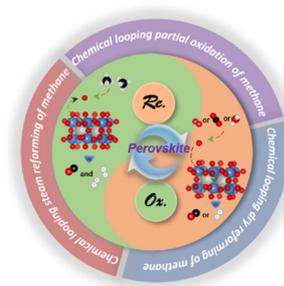
Mathias Rapacioli,\* Maysa Yusef Buey and Fernand Spiegelman



1516

### Perovskites as oxygen storage materials for chemical looping partial oxidation and reforming of methane

Yuelun Li, Mingyi Chen, Lei Jiang, Dong Tian\* and Kongzhai Li\*



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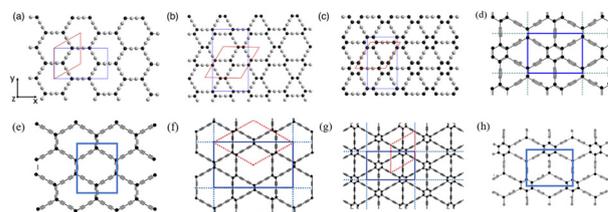
Fundamental questions  
Elemental answers

## REVIEWS

1541

## Graphyne and graphdiyne nanoribbons: from their structures and properties to potential applications

Qiaohan Liu, Xiaorong Wang, Jing Yu\* and Jingang Wang\*

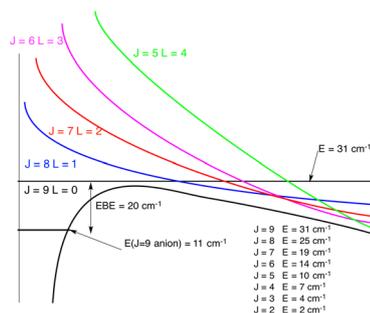


## PERSPECTIVES

1564

## An environmental impact statement for molecular anions

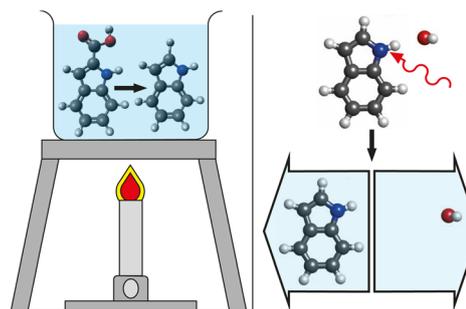
Jack Simons



1587

## Unraveling the ultrafast dynamics of thermal-energy chemical reactions

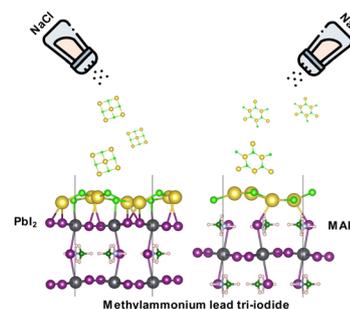
Matthew S. Robinson and Jochen Küpper\*



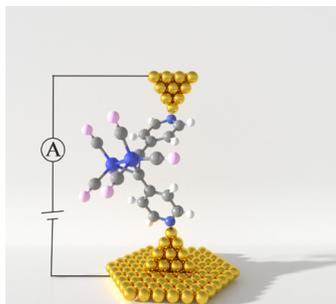
## COMMUNICATIONS

1602

## Exotic hexagonal NaCl atom-thin layer on methylammonium lead iodide perovskite: new hints for perovskite solar cells from first-principles calculations

Adriana Pecoraro, Ana B. Muñoz-García,\*  
Gennaro V. Sannino, Paola Delli Veneri and Michele Pavone\*

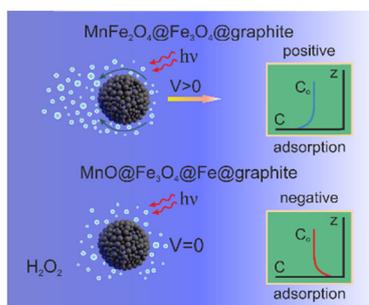
1608



### Manipulating the charge transport *via* incorporating a cobalt bridge into a single-molecule junction

Chaoqi Ma, Yunpeng Li, Ajun Tang, Rui Wang, Yingjie Li, Zhi Li, Jiawei Yang and Hongxiang Li\*

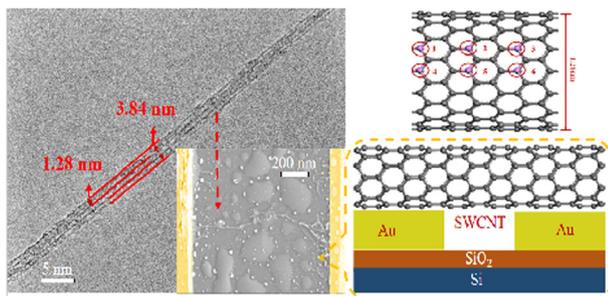
1612



### The role of self-diffusiophoresis and reactive force during the propulsion of manganese-based catalytic micromotors

Boris Kichatov,\* Alexey Korshunov, Vladimir Sudakov, Alexandr Golubkov, Dmitriy Smovzh,\* Salavat Sakhapov and Mikhail Skirda

1616



### Single walled carbon nanotubes band gap width measurement and the influence of nitrogen doping research

Rui Miao, Yujian Liang, Guangfeng Zhou, Yayu Deng, Lei Wang, Jingui Deng and Qingyi Shao\*

1625



### Hydration deactivation mechanism of the $\langle 100 \rangle$ oriented cuprous oxide photocathodes in solar water splitting and the regenerated three-dimensional structure

Yang Li,\* Jiating Wu, Yuhe Zheng, Yajing Fan, Ting Bian, Xinyu Fan, Santana Vimbai Masendu, Junhua Xu and Zongping Shao\*

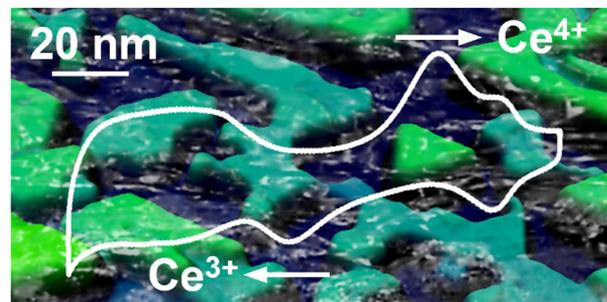


## RESEARCH PAPERS

1630

**A model study of ceria–Pt electrocatalysts: stability, redox properties and hydrogen intercalation**

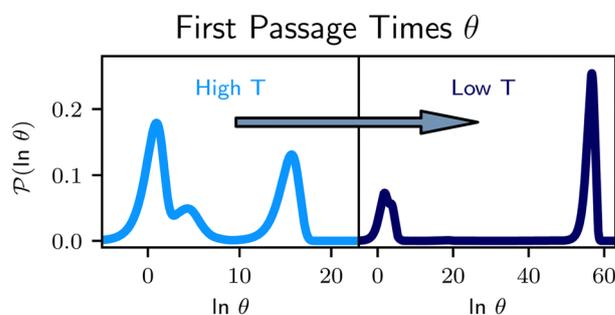
Lukáš Fusek, Pankaj Kumar Samal, Jiří Keresteš, Ivan Khalakhan, Viktor Johánek, Yaroslava Lykhach, Jörg Libuda, Olaf Brummel\* and Josef Mysliveček\*



1640

**Analysis and interpretation of first passage time distributions featuring rare events**

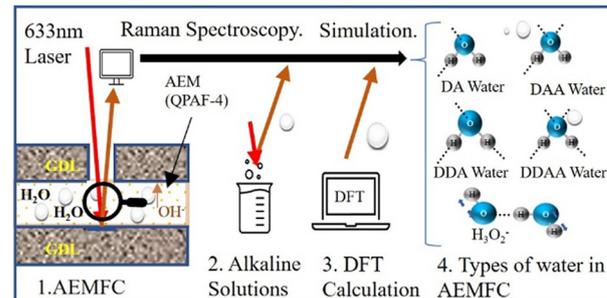
Esmæ J. Woods and David J. Wales\*



1658

**Various states of water species in an anion exchange membrane characterized by Raman spectroscopy under controlled temperature and humidity**

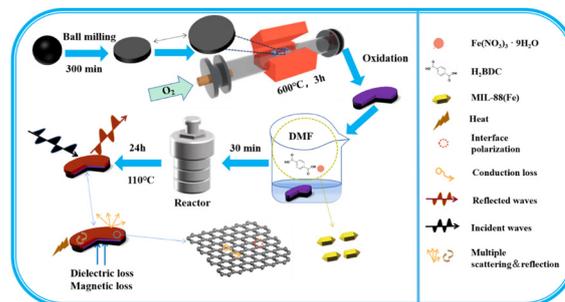
Solomon Wekesa Wakolo, Donald A. Tryk, Hiromichi Nishiyama, Kenji Miyatake, Akihiro Iiyama and Junji Inukai\*



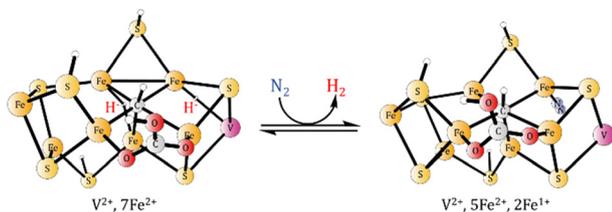
1671

**Preparation of MIL-88(Fe)@Fe<sub>2</sub>O<sub>3</sub>@FeSiCr double core–shell-structural composites and their wave-absorbing properties**

Wenmiao Zhang, Hongzhang Du, Lei Wang,\* Sajjad Ur Rehman, Shuqi Shen, Weiwei Dong, Yifeng Hu, Haiping Zou\* and Tongxiang Liang



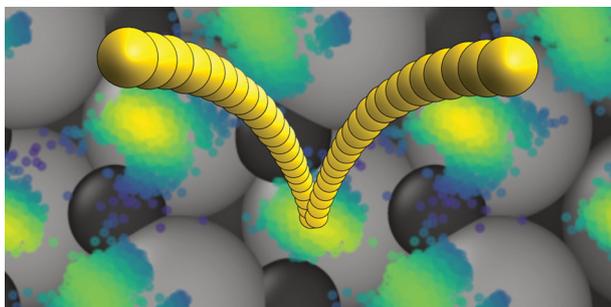
1684



### The energetics of $N_2$ reduction by vanadium containing nitrogenase

Per E. M. Siegbahn\* and Wen-Jie Wei

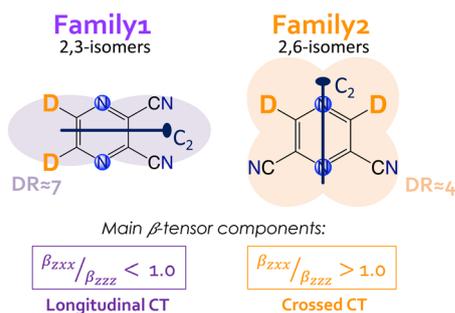
1696



### Hydrogen atom scattering at the $Al_2O_3(0001)$ surface: a combined experimental and theoretical study

Martin Liebetrau, Yvonne Dorenkamp, Oliver Bünermann\* and Jörg Behler\*

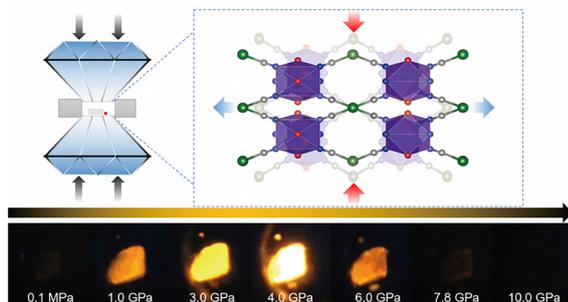
1709



### Second-order nonlinear optical properties of X-shaped pyrazine derivatives

Verónica Postils,\* Zuzana Burešová, David Casanova, Benoît Champagne, Filip Bureš, Vincent Rodriguez\* and Frédéric Castet\*

1722



### Negative linear compressibility and strong enhancement of emission in $Eu[Ag(CN)_2]_3 \cdot 3H_2O$ under pressure

Yu Liu, Boyang Fu, Min Wu, Weilong He, Donghua Liu,\* Fuyang Liu, Luhong Wang, Haozhe Liu, Kai Wang and Weizhao Cai\*

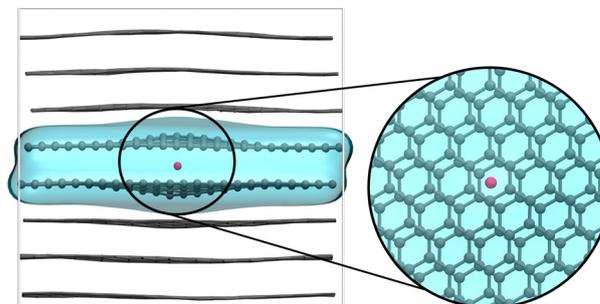


## RESEARCH PAPERS

1729

## Towards hybrid quantum mechanical/molecular mechanical simulations of Li and Na intercalation in graphite – force field development and DFTB parametrisation

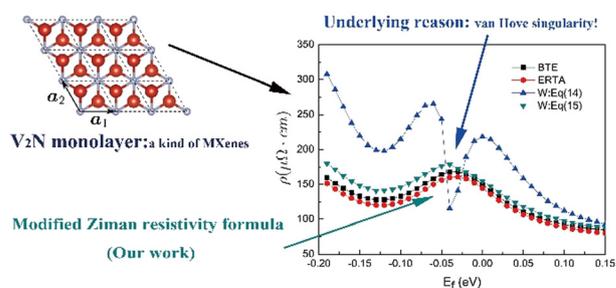
Felix R. S. Purtscher and Thomas S. Hofer\*



1741

First-principles calculations on the intrinsic resistivity of realistic metals: a case study of monolayer  $V_2N$ 

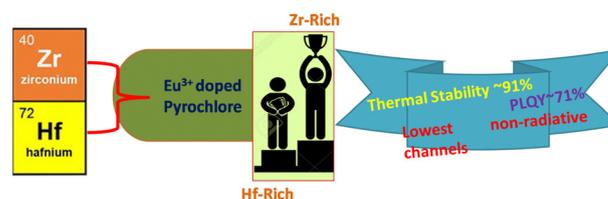
Binyuan Zhang and Weijiang Gong\*



1749

Composition-dependent photoluminescence in nanocrystalline  $La_2Hf_{2-x}Zr_xO_7:Eu$  phosphor: role of chemical twin Zr/Hf environments around a luminescent center

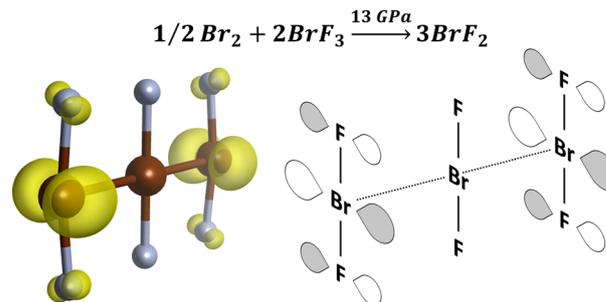
Santosh K. Gupta,\* Sandeep Nigam and Yuanbing Mao



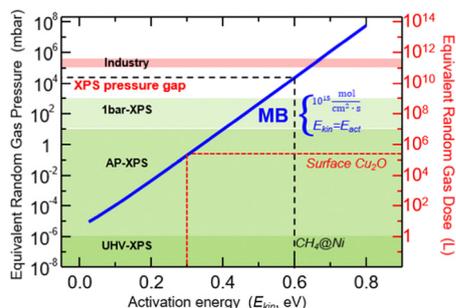
1762

## High-pressure stabilization of open-shell bromine fluorides

Madhavi H. Dalsaniya,\* Deepak Upadhyay, Krzysztof Jan Kurzydowski and Dominik Kurzydowski\*



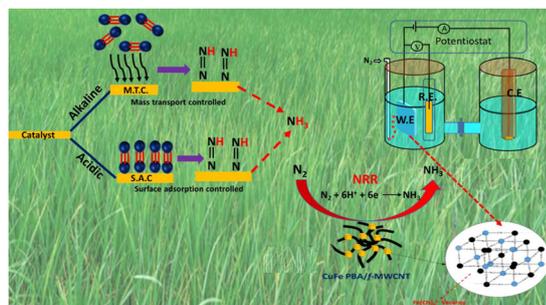
1770



### Simulating high-pressure surface reactions with molecular beams

Amjad Al Taleb, Frederik Schiller, Denis V. Vyalikh, José María Pérez, Sabine V. Auras, Daniel Farias and J. Enrique Ortega\*

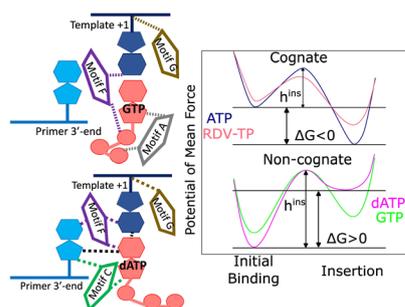
1777



### Mechanistic insights into the electrolyte effects on the electrochemical nitrogen reduction reaction using copper hexacyanoferrate/f-MWCNT nano-composites

Aamir Y. Bhat, Priya Jain, Mohsin A. Bhat and Pravin P. Ingole\*

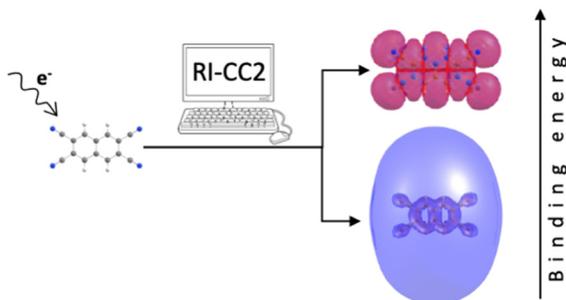
1792



### Trapping a non-cognate nucleotide upon initial binding for replication fidelity control in SARS-CoV-2 RNA dependent RNA polymerase

Moises E. Romero, Shannon J. McElhenney and Jin Yu\*

1809



### On the performance of second-order approximate coupled-cluster singles and doubles methods for non-valence anions

Garrette Pauley Paran, Cansu Utku and Thomas-Christian Jagau\*



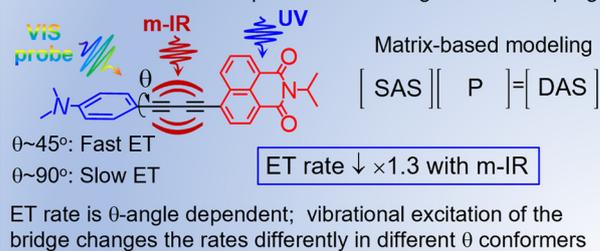
## RESEARCH PAPERS

1819

### Electron transfer rate modulation with mid-IR in butadiyne-bridged donor–bridge–acceptor compounds

Kasun C. Mendis, Xiao Li, Jesús Valdiviezo, Susannah D. Banziger, Peng Zhang, Tong Ren, David N. Beratan and Igor V. Rubtsov\*

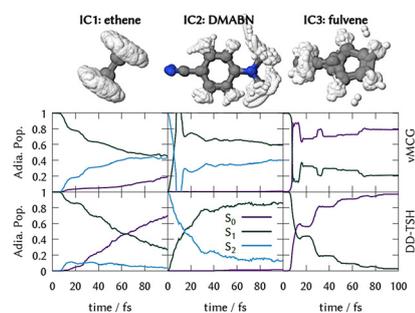
ET rate modulation in the presence of strong vibronic coupling



1829

### Benchmarking non-adiabatic quantum dynamics using the molecular Tully models

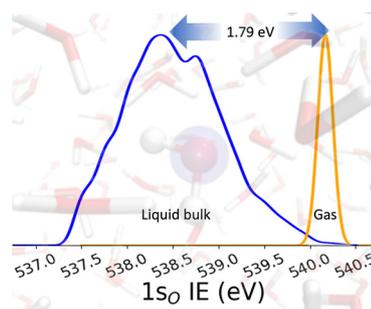
Sandra Gómez, Eryn Spinlove and Graham Worth\*



1845

### Core-ionization spectrum of liquid water

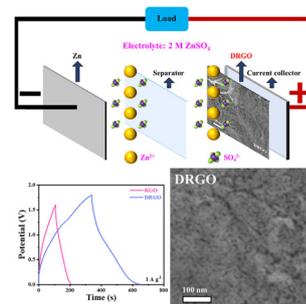
Sourav Dey, Sarai Dery Folkestad, Alexander C. Paul, Henrik Koch and Anna I. Krylov\*



1860

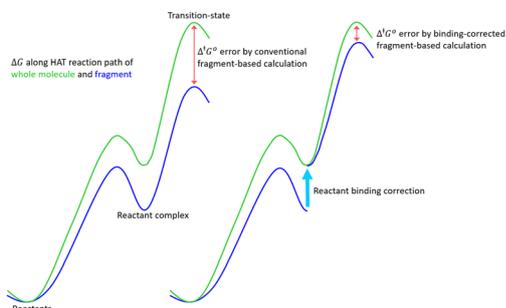
### High-energy-density zinc ion capacitors based on 3D porous free-standing defect-reduced graphene oxide hydrogel cathodes

Peng Liao, Xiang Yu, Jiaqi He,\* Xin Zhang, Wenjie Yan, Zenghui Qiu\* and Haijun Xu\*



## RESEARCH PAPERS

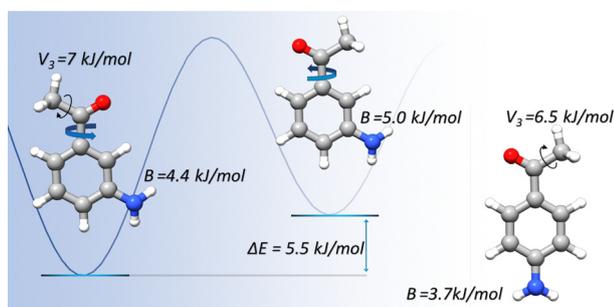
1869



### Robust fragment-based method of calculating hydrogen atom transfer activation barrier in complex molecules

Yizhou Liu,\* Frank C. Pickard IV, Gregory W. Sluggett and Iason G. Mustakis

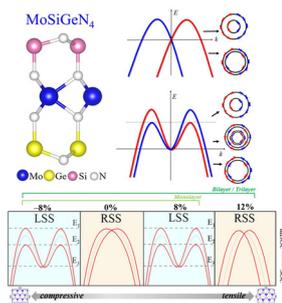
1881



### Structure and dynamics of 3'-aminoacetophenone and 4'-aminoacetophenone from rotational spectroscopy

Giovanna Salvitti, Silvia Sigismondi, Sonia Melandri, Juan Carlos López, Susana Blanco\* and Assimo Maris\*

1891

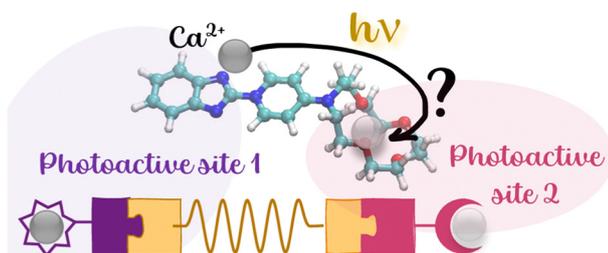


### Biaxial strain modulated electronic structures of layered two-dimensional MoSiGeN<sub>4</sub> Rashba systems

Puxuan Li, Xuan Wang, Haoyu Wang, Qikun Tian, Jinyuan Xu, Linfeng Yu, Guangzhao Qin\* and Zhenzhen Qin\*

1904

### Excited State Cation transfer



### *In silico* strategy to design an efficient organic photoswitch based on excited-state cation transfer

Laure de Thieulloy, Cédric Mongin, Isabelle Leray, Clément Guerrin, Guy Buntinx, Stéphane Aloïse and Aurélie Perrier\*

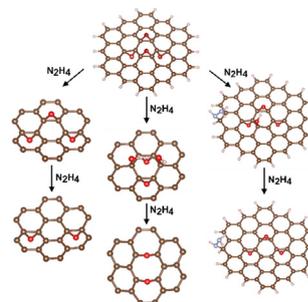


## RESEARCH PAPERS

1917

## Exploring the mechanism of graphene-oxide reduction by hydrazine in a multi-epoxide environment with DFT calculations

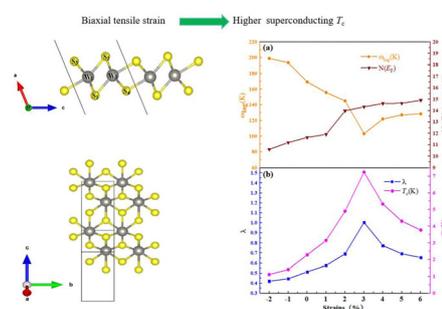
Nguyen Tri Hieu, Dénes Szieberth and Eszter Makkos\*



1929

First-principles prediction of superconducting properties of monolayer 1T'-WS<sub>2</sub> under biaxial tensile strain

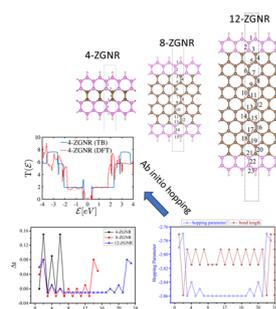
Guo-Hua Liu, Shu-Xiang Qiao, Qiu-Hao Wang, Hao Wang, Hao-Dong Liu, Xin-Zhu Yin, Jin-Han Tan, Na Jiao, Hong-Yan Lu\* and Ping Zhang\*



1936

Influence of *ab initio* derived site-dependent hopping parameters on electronic transport in graphene nanoribbons

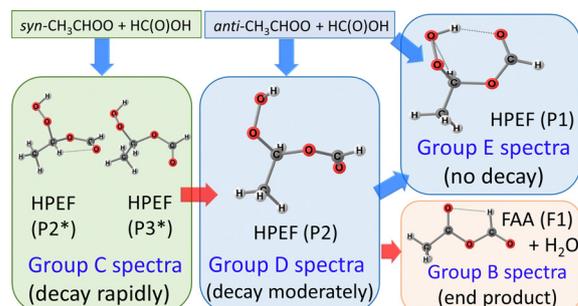
Masoumeh Davoudiniya, Bo Yang and Biplab Sanyal\*



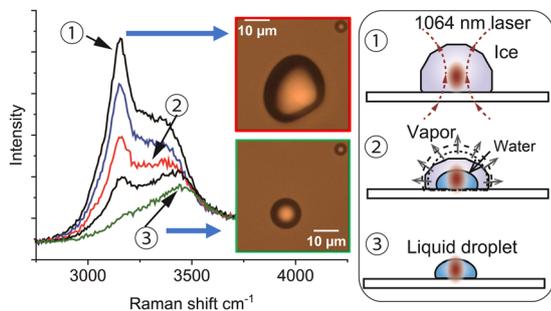
1950

Detailed mechanism and kinetics of reactions of *anti*- and *syn*-CH<sub>3</sub>CHOO with HC(O)OH: infrared spectra of conformers of hydroperoxyethyl formate

Bedabyas Behera and Yuan-Pern Lee\*



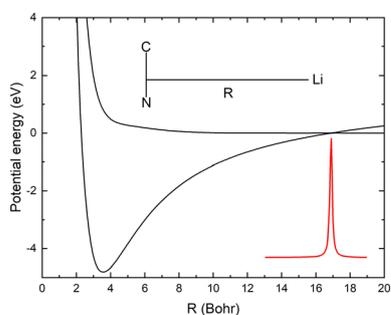
1967



### Melting of a single ice microparticle on exposure to focused near-IR laser beam to yield a supercooled water droplet

Shuichi Hashimoto\* and Takayuki Uwada

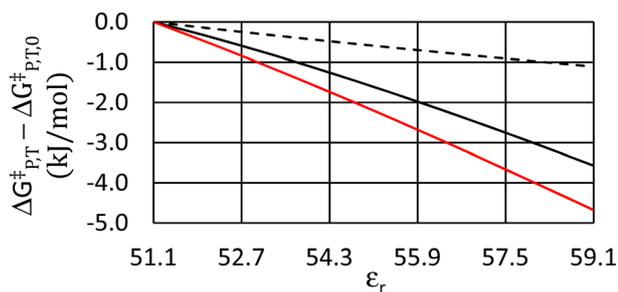
1977



### Mutual neutralization in collisions of $\text{Li}^+$ with $\text{CN}^-$

Åsa Larson\* and Ann E. Orel

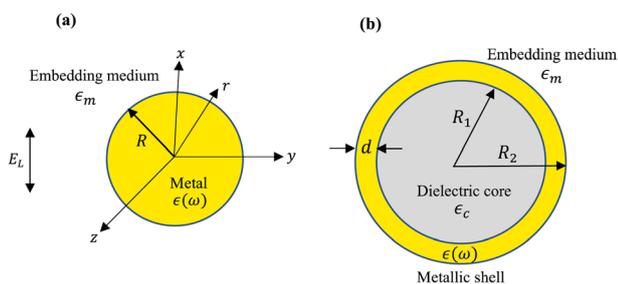
1984



### A thermodynamic approach to analyzing relative permittivity and solvent mole fraction models, and application to $\text{S}_{\text{N}}1$ reactions

Floyd L. Wiseman\* and Dane W. Scott

1994



### Bandwidth of quantized surface plasmons: competition between radiative and nonradiative damping effects

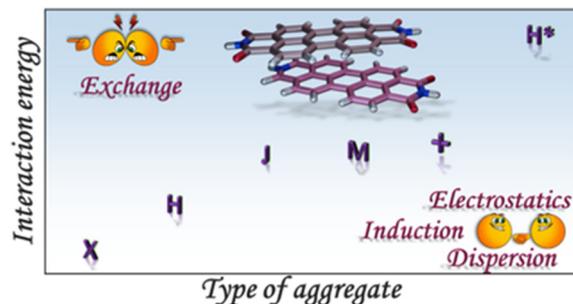
Samar Moustafa, Mohamed K. Zayed, Moustafa Ahmed and Hesham Fares\*



2007

### Energy landscape of perylene-3,4,9,10-tetracarboxylic diimide chromophoric aggregates

Pallavi Panthakal Das, Aniruddha Mazumder, Megha Rajeevan, Rotti Srinivasamurthy Swathi\* and Mahesh Hariharan\*



2016

### Exploring the impact of alignment media on RDC analysis of phosphorus-containing compounds: a molecular docking approach

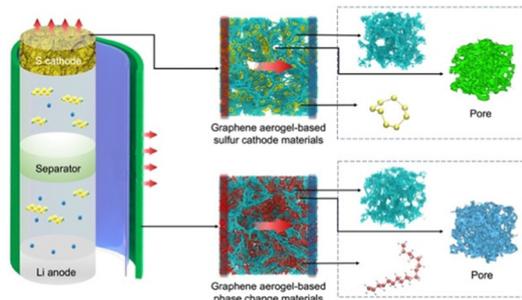
Markéta Christou Tichotová, Lucie Tučková, Hugo Kocek, Aleš Růžička, Michal Straka and Eliška Procházková\*



2025

### Thermal transport properties of graphene aerogel as an advanced carrier for enhanced energy storage

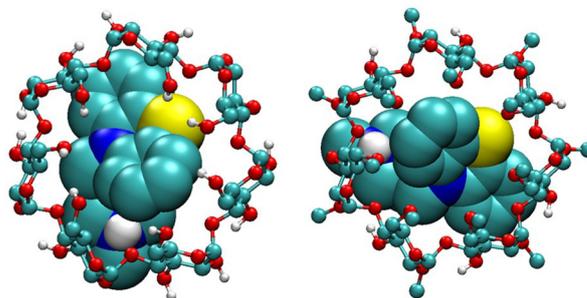
Jieren Song,\* Xianghua Xu and Xingang Liang



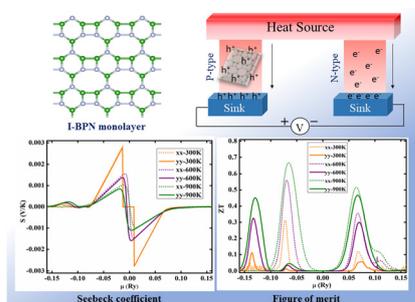
2035

### Host-guest systems for the SAMPL9 blinded prediction challenge: phenothiazine as a privileged scaffold for binding to cyclodextrins

Brenda Andrade, Ashley Chen and Michael K. Gilson\*



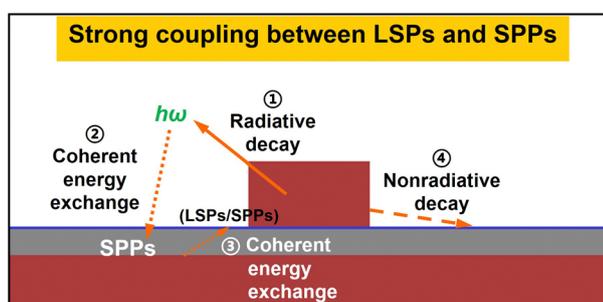
2044



### Theoretical insights into the structural, electronic and thermoelectric properties of the inorganic biphenylene monolayer

Ajay Kumar, Parbati Senapati and Prakash Parida\*

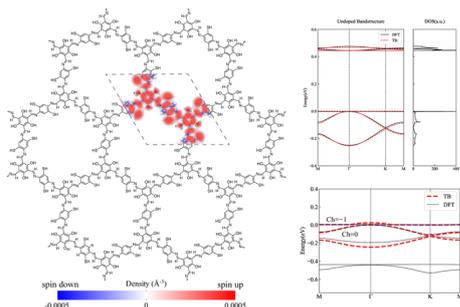
2058



### Tailoring linear and nonlinear plasmons of metal/MoS<sub>2</sub>/metal nanostructures

Shuangqing Jiang, Zonglin Li, Jingwu Tang,\*  
Wen Huang, Zanxian Tan, Dingyu Pan, Xiyang Chen and Guozheng Nie\*

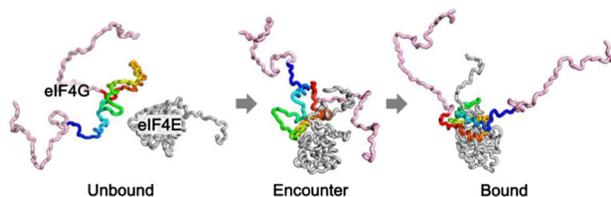
2066



### Enantiomeric kagome bands in a two-dimensional covalent organic framework with non-trivial magnetic and topological properties

Quan Gao, Xuelian Sun, Xuhui Xu, Xinxin Jiang,  
Zhikuan Wang, Lei Yang, Dongmei Li, Bin Cui\* and  
Desheng Liu\*

2073



### Molecular dynamics simulations revealed topological frustration in the binding-wrapping process of eIF4G with eIF4E

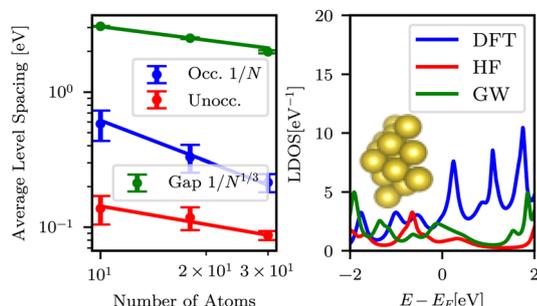
Meng Gao and Yongqi Huang\*





## RESEARCH PAPERS

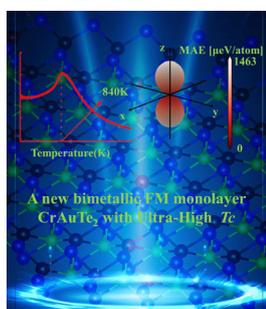
2127



### Widening of the fundamental gap in cluster GW for metal–molecular interfaces

Štěpán Marek\* and Richard Korytár

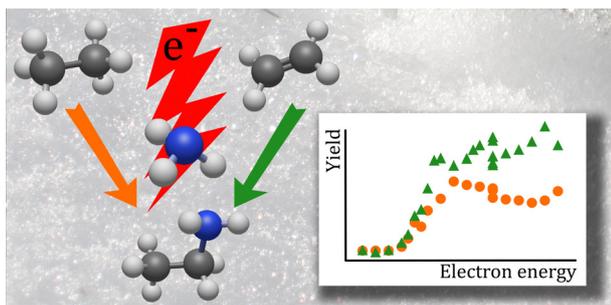
2134



### Toward intrinsic ultra-high-temperature ferromagnetism in a CrAuTe<sub>2</sub>/graphene heterosystem

Chaobin Jia, Chao Jin, Puyuan Shi, Jingjuan Su, Yungeng Zhang,\* Xianghong Niu\* and Bing Wang\*

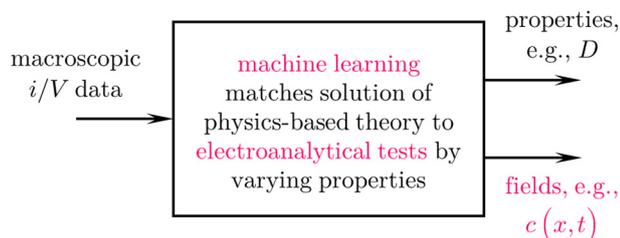
2140



### Electron-induced hydroamination of ethane as compared to ethene: implications for the reaction mechanism

Hannah Boeckers, Martin Philipp Mues, Jan Hendrik Bredehöft and Petra Swiderek\*

2153



### How machine learning can extend electroanalytical measurements beyond analytical interpretation

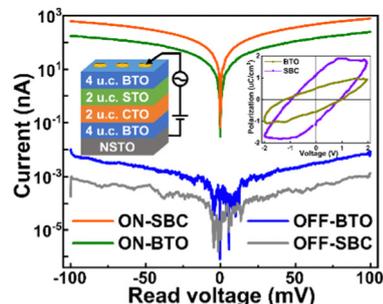
Aashutosh Mistry,\* Ian D. Johnson, Jordi Cabana, Brian J. Ingram\* and Venkat Srinivasan\*



2168

### Giant tunnel resistance effect in $(\text{SrTiO}_3)_2/(\text{BaTiO}_3)_4/(\text{CaTiO}_3)_2$ asymmetric superlattice with enhanced polarization

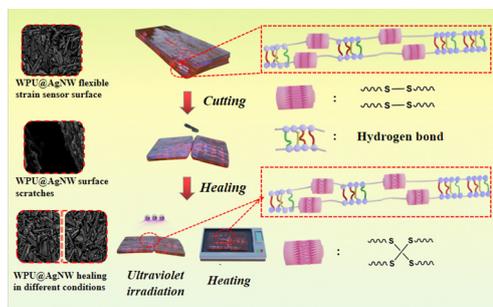
Xiubing Zhang, Haoming Wei,\* Yangqing Wu, Tengzhou Yang and Bingqiang Cao\*



2175

### Multifunctional aqueous polyurethanes with high strength and self-healing efficiency based on silver nanowires for flexible strain sensors

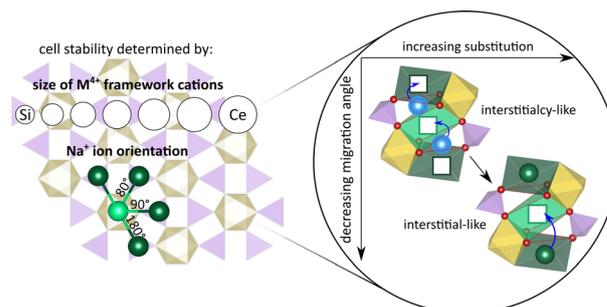
Haibin Niu, Jiaqi Li, Xin Song, Kaiyang Zhao, Li Liu,\* Chao Zhou and Guangfeng Wu\*



2190

### Interstitial or interstitialcy: effect of the cation size on the migration mechanism in NaSiCON materials

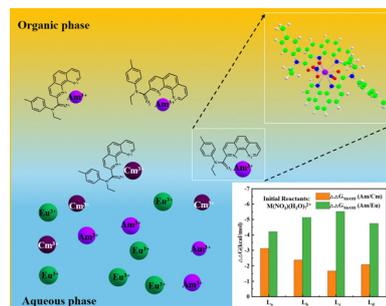
Judith Schuett, Johanna Schillings and Steffen Neitzel-Grieshammer\*



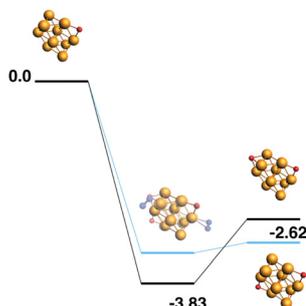
2205

### Theoretical investigations into the bonding and separation properties of non-rigid, partially rigid, and rigid ligands derived from Et-Tol-PTA with trivalent lanthanides and actinides

Shouqiang Wu and An Yong Li\*



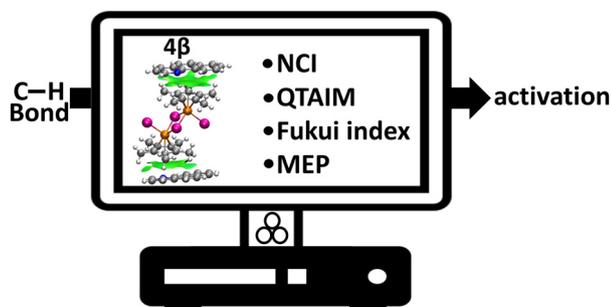
2218



### Reactions of $N_2O$ and $CO$ on neutral $Rh_{10}O_n$ clusters: a density functional study

Vikram Muman, Alex Tennyson-Davies, Oihan Allegret and Matthew A. Addicoat\*

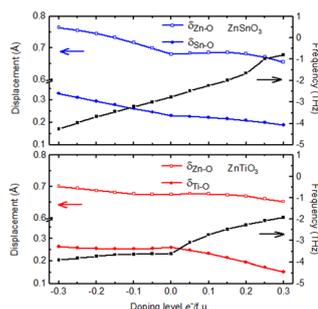
2228



### Interactions and reactivity in crystalline intermediates of mechanochemical cyclorhodation reactions

Sara Gómez,\* Santiago Gómez, Natalia Rojas-Valencia, José G. Hernández, Karen J. Ardila-Fierro, Tatiana Gómez, Carlos Cárdenas, Cacier Hadad, Chiara Cappelli and Albeiro Restrepo\*

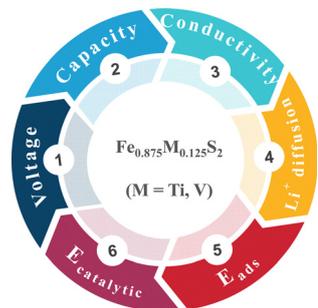
2242



### Comparison of carrier doping in $ZnSnO_3$ and $ZnTiO_3$ from first principles

Jing Li, Jing Su, Qing Zhang, Changfeng Fang\* and Xiaohui Liu\*

2249



### First-principles study of the discharge electrochemical and catalytic performance of the sulfur cathode host $Fe_{0.875}M_{0.125}S_2$ ( $M = Ti, V$ )

Cheng-Dong Wei, Hong-Tao Xue, Yu-Xia Hu, Qing-Shan Zhao and Fu-Ling Tang\*

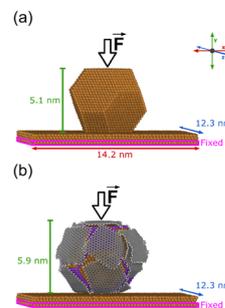


## RESEARCH PAPERS

2260

## On the mechanical response of graphene-capped copper nanoparticles

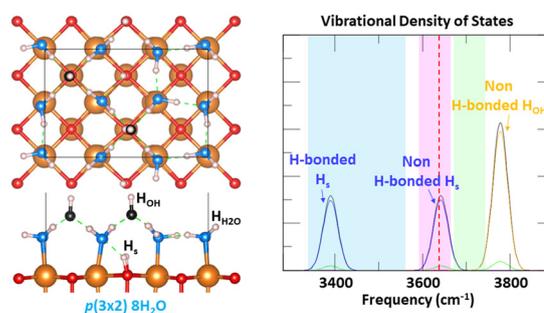
Gabriel J. Olguín-Orellana, Juan A. de la Rosa Abad, María B. Camarada, Sergio J. Mejía-Rosales, Jans Alzate-Morales and Marcelo M. Mariscal\*



2269

## First principles simulations of MgO(100) surface hydration at ambient conditions

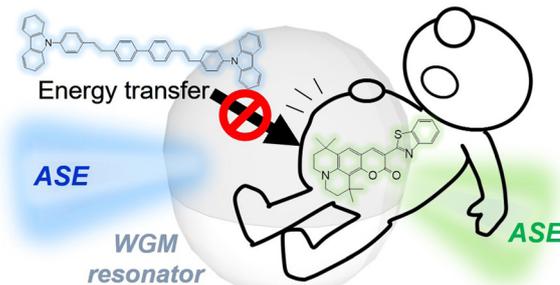
Michel Sassi\* and Kevin M. Rosso



2277

## Device parameter to evaluate exciton energy transfer in organic whispering-gallery-mode microresonators and its dependence on the amplified spontaneous emission threshold

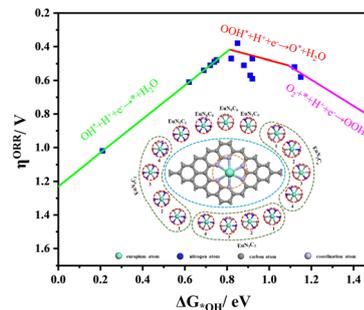
Tomoki Mikajiri, Takeshi Komino,\* Jun-ichi Yamada and Hiroyuki Tajima



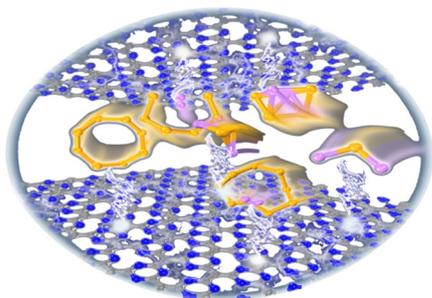
2284

## Mechanistic study of Eu single atoms occupying four vacancy centers as potential electrocatalysts for the oxygen reduction reaction

Qiming Fu, Daomiao Wang\* and Chao Liu\*



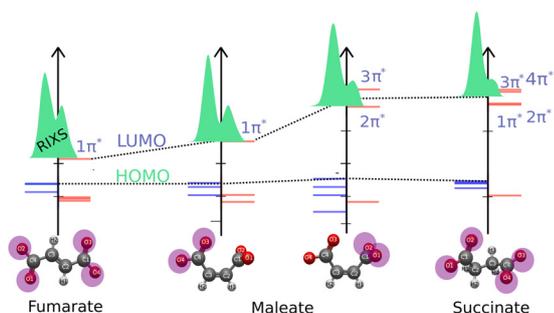
2291



### Anchoring and catalytic insights into bilayer $C_4N_3$ material for lithium–selenium batteries: a first-principles study

Zehui Yang, Wentao Liu, Shulin Bai, Peng Ai, Hao Wang, Tuo Zheng, Qingshun Li and Shuwei Tang\*

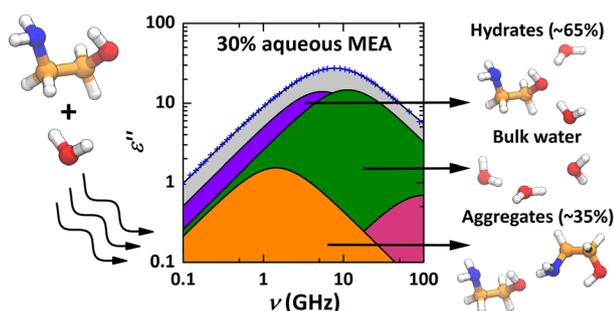
2304



### Electronic structure, bonding and stability of fumarate, maleate, and succinate dianions from X-ray spectroscopy

Viktoriia Savchenko,\* Sebastian Eckert, Mattis Fondell, Rolf Mitzner, Vincius Vaz da Cruz and Alexander Föhlisch

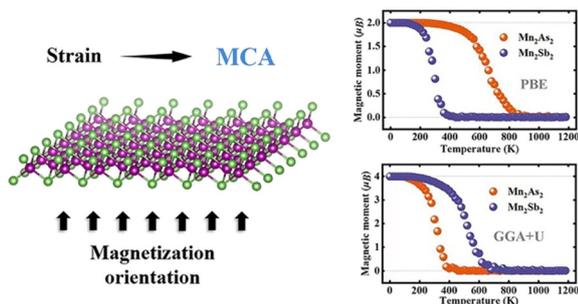
2312



### What is behind a gas stream scrubbing liquid? Monoethanolamine/water mixtures as seen by dielectric relaxation spectroscopy

Vira Agjeienko\* and Richard Buchner

2324



### Theoretical prediction of two-dimensional ferromagnetic $Mn_2X_2$ ( $X = As, Sb$ ) with strain-controlled magnetocrystalline anisotropy

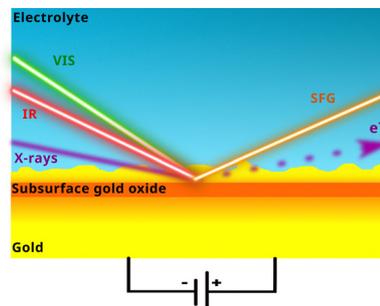
Yi Zhao, Zesen Lei, Yonghao Wang, Wei Yan,\* Ruishan Tan, Tao Jing and Qilong Sun\*



2332

### Multi-spectroscopic study of electrochemically-formed oxide-derived gold electrodes

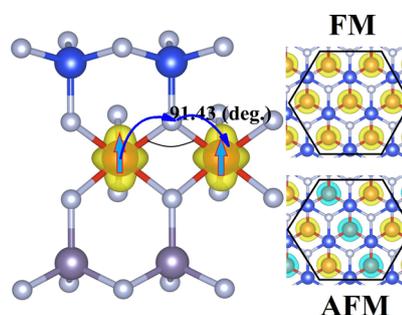
Sara Boscolo Bibi, Ahmed M. El-Zohry,\*  
Bernadette Davies, Vladimir Grigorev,  
Christopher M. Goodwin, Patrick Lömker,  
Alexander Holm, Harri Ali-Löytty,  
Fernando Garcia-Martinez, Christoph Schlueter,  
Markus Soldemo, Sergey Koroidov\* and Tony Hansson\*



2341

### Tunable polarization properties of charge, spin, and valley in Janus VSiGeZ<sub>4</sub> (Z = N, P, As) monolayers

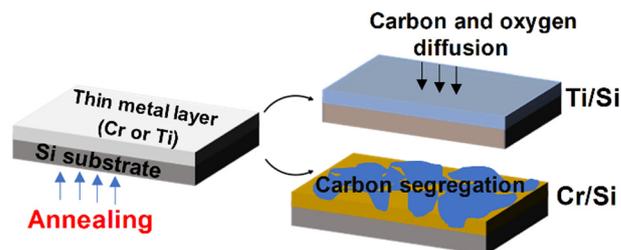
Ming-Yang Liu,\* Guang-Qiang Li, Yao He and Kai Xiong



2355

### Enhancing electrocatalytic activity in metallic thin films through surface segregation of carbon

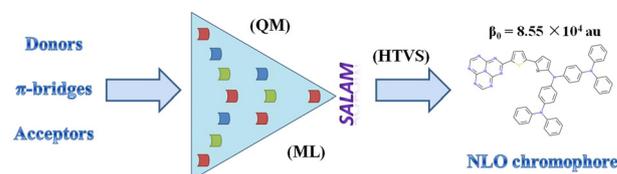
Ayesha Kousar, Ulviyya Quliyeva, Ishan Pande,  
Jani Sainio, Jaakko Julin, Timo Sajavaara,  
Antti J. Karttunen and Tomi Laurila\*



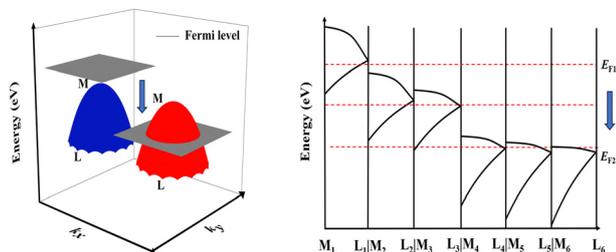
2363

### High-throughput virtual screening of organic second-order nonlinear optical chromophores within the donor- $\pi$ -bridge-acceptor framework

Chunyun Tu,\* Weijiang Huang, Sheng Liang, Kui Wang,  
Qin Tian and Wei Yan\*



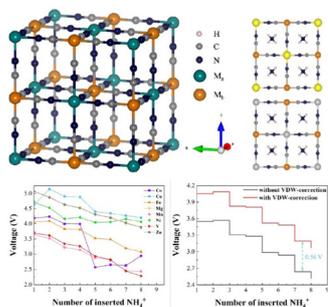
2376



### Theoretical study of CDW phases for bulk NbX<sub>2</sub> (X = S and Se)

Hongwei Du, Zhenyi Jiang,\* Jiming Zheng,\*  
Xiaodong Zhang, Wenxuan Wang and Zhiyong Zhang

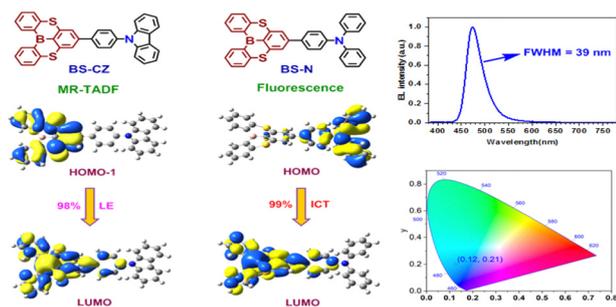
2387



### Element screening of metal sites in Fe-based Prussian blue framework materials for ammonium ion battery applications: a first-principles study

Yu Zhang, Junjie Xing, Bo Zhang, Likai Tong and  
Xiuli Fu\*

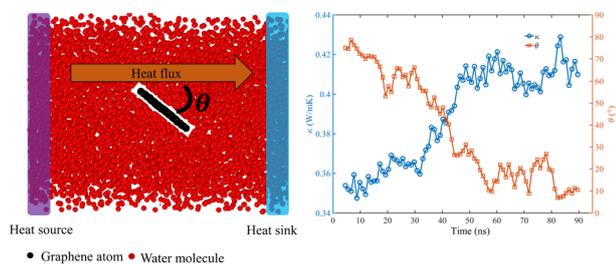
2395



### B-embedded disulfide-bridged $\pi$ -conjugated compounds: structures and optical tuning

Kaishun Ye, Gang Li, Feiyang Li, Chao Shi,\* Zhen Jiang,  
Fuzheng Zhang, Qiuxia Li,\* Jie Su, Dandan Song\* and  
Aihua Yuan

2402



### Coupling at the molecular scale between the graphene nanosheet and water and its effect on the thermal conductivity of the nanofluid

Xiong Pan, Hanhui Jin,\* Xiaoke Ku, Yu Guo and  
Jianren Fan

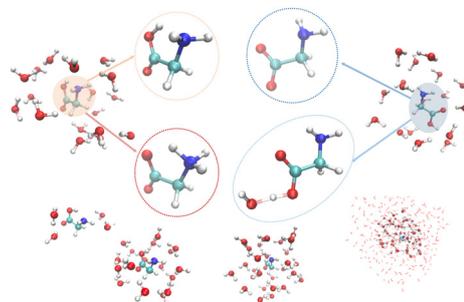


## RESEARCH PAPERS

2414

**Temperature driven transformations of glycine molecules embedded in interstellar ice**

Maysa Yusef-Buey, Tzonka Mineva, Dahbia Talbi and Mathias Rapacioli\*



2426

**Boiling, critical, and freezing temperatures in light of molecular descriptors: correlation and causation**

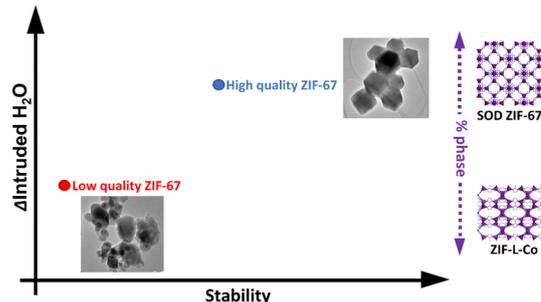
Ossama Abdeen, Mohamed Ismael\* and Aly Abdou\*



2440

**Quality-dependent performance of hydrophobic ZIF-67 upon high-pressure water intrusion–extrusion process**

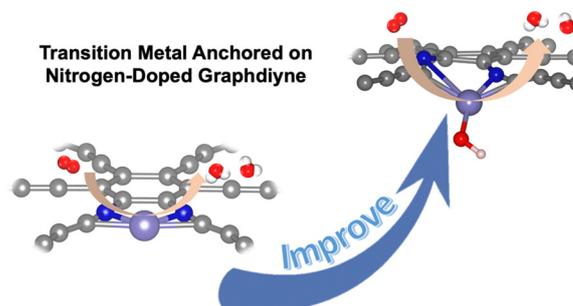
Eder Amayuelas,\* Luis Bartolomé, Yan Zhang, Juan Miguel López del Amo, Oleksandr Bondarchuk, Artem Nikulin, Francisco Bonilla, Elena Palomo del Barrio, Paweł Zajdel\* and Yaroslav Grosu\*



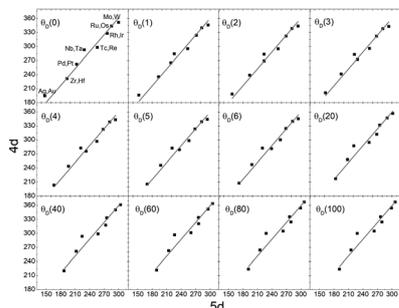
2449

**Transition metals anchored on nitrogen-doped graphdiyne for an efficient oxygen reduction reaction: a DFT study**

Ning Wang, Siyu Gan, Yunfeng Mao, Junping Xiao,\* Chunming Xu and Tianhang Zhou\*



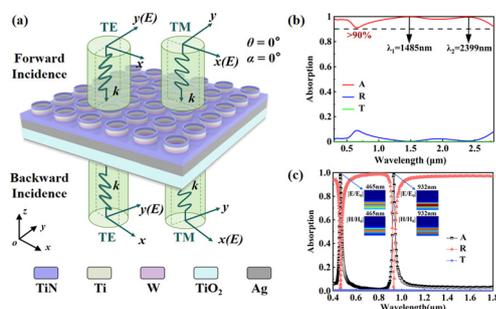
2457



## Vibrational and cohesive properties in 4d and 5d transition metals: systematics and interrelations

Dalia S. Bertoldi\* and A. Fernández Guillermet

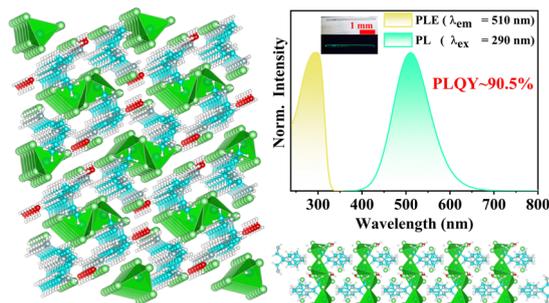
2463



## A multifunctional switching bidirectional optical absorber based on a titanium nitride metamaterial

Lijing Su, Hengli Feng, Pengfei Sun, Yaxin Zhou, Xin Li, Sihan Nie, Lingling Ran and Yang Gao\*

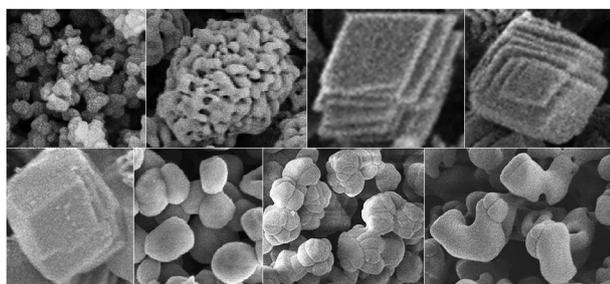
2472



## A zero-dimensional hybrid copper(I) bromide single crystal with highly efficient green emission

Yingui Gao, Zhihuang Xu, Liwang Ye, Yuanjie Wang and Xinxin Zhuang\*

2478



## Morphologies and magnetic properties of $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> nanoparticles calcined at different temperatures

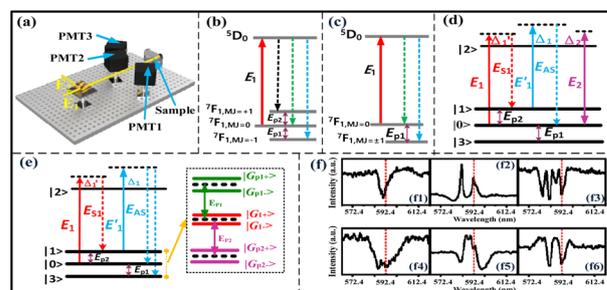
Xue-Min He, Duan-Qing Chen, Kun-Yu Su, Zhen-Fei Yu, Yi Zhang and Wei Zhong\*



2486

### Spectral and temporal atomic coherence interaction in $\text{Eu}^{3+}:\text{NaYF}_4$ and $\text{Eu}^{3+}:\text{BiPO}_4$

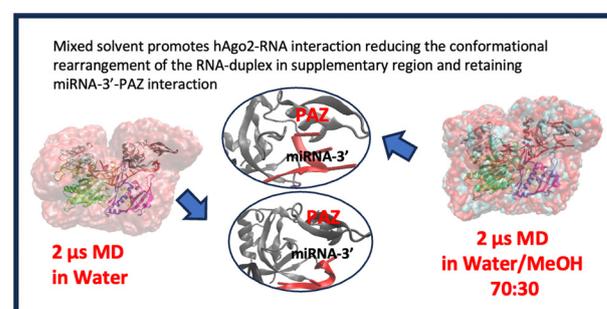
Zhou Feng, Muhammad Imran, Faisal Nadeem, Huanrong Fan, Jin Yan, Irfan Ahmed, Condon Lau\* and Yanpeng Zhang\*



2497

### Probing the conformational dynamics of an Ago-RNA complex in water/methanol solution

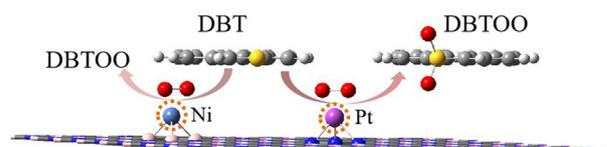
Francesco Porcelli, Anna Rita Casavola, Alessandro Grottesi, Donatella Schiumarini and Lorenzo Avaldi



2509

### The single metal atom (Ni, Pd, Pt) anchored on defective hexagonal boron nitride for oxidative desulfurization

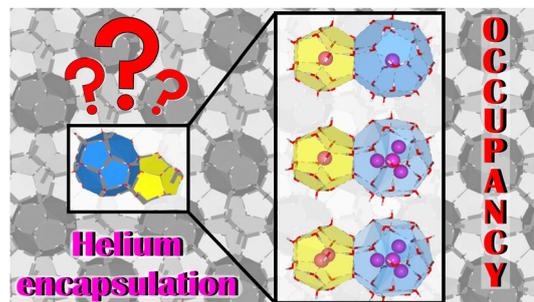
Naixia Lv, Hongshun Ran, Jinrui Zhang, Jie Yin, Yuan Zhang, Hongping Li\* and Linhua Zhu\*



2519

### Analysing the stability of He-filled hydrates: how many He atoms fit in the sII crystal?

Raquel Yanes-Rodríguez and Rita Prosimiti\*



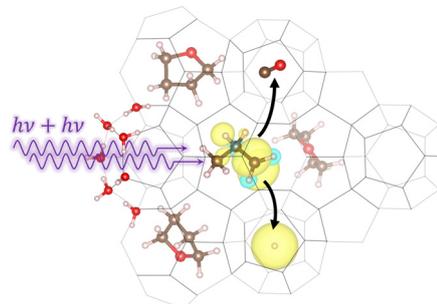


## RESEARCH PAPERS

2568

**Two-photon chemistry of tetrahydrofuran in clathrate hydrates**

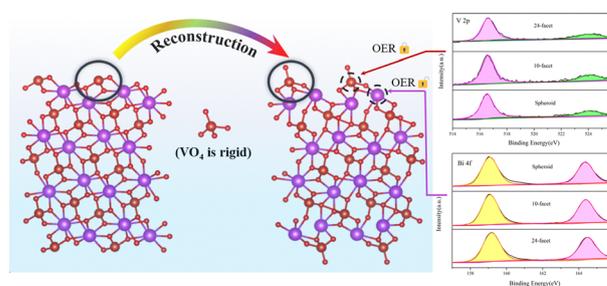
Michael A. Michon,\* Pawel Chmielniak, Peter M. Weber\* and Christoph Rose-Petruck\*



2580

**Oxygen evolution reaction (OER) active sites in BiVO<sub>4</sub> studied using density functional theory and XPS experiments**

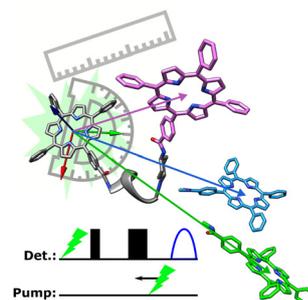
Qingyan Zhang, Guowei Liu and Taifeng Liu\*



2589

**Determining and controlling conformational information from orientationally selective light-induced triplet-triplet electron resonance spectroscopy for a set of bis-porphyrin rulers**

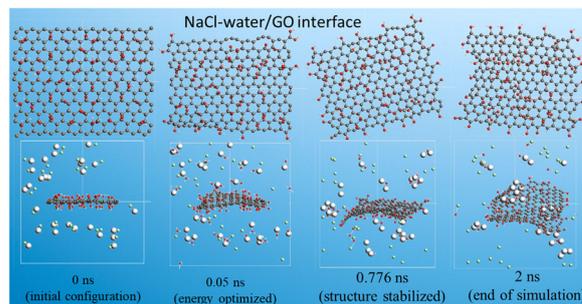
Arnau Bertran,\* Marta De Zotti, Christiane R. Timmel, Marilena Di Valentin\* and Alice M. Bowen\*



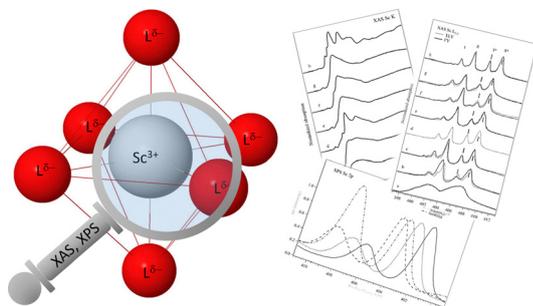
2603

**ReaxFF molecular dynamics of graphene oxide/NaCl aqueous solution interfaces**

Rokhsareh Akbarzadeh and Milan Pěrdota\*



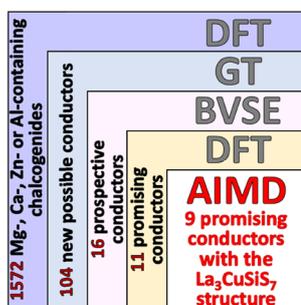
2613



### Chemical bonding effects in Sc compounds studied using X-ray absorption and X-ray photoelectron spectroscopies

Anna Zimina,\* Aline Léon and Ralph Steininger

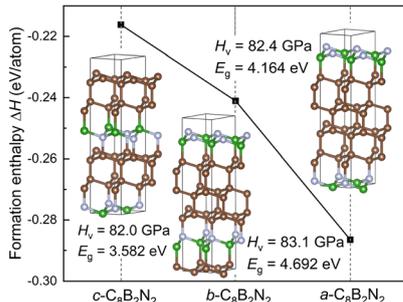
2622



### A novel class of multivalent ionic conductors with the $\text{La}_3\text{CuSi}_5$ structure type: results of stepwise ICSD screening

Artem A. Kabanov,\* Yelizaveta A. Morkhova,\* Vladislav T. Osipov, Manuel Rothenberger, Tilmann Leisegang and Vladislav A. Blatov

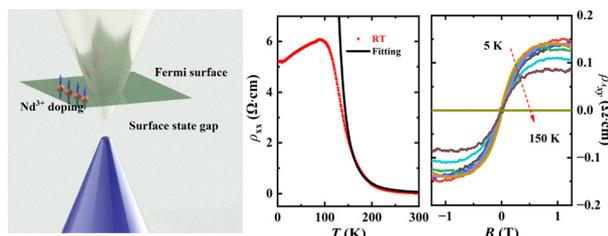
2629



### Novel superhard semiconducting structures of $\text{C}_8\text{B}_2\text{N}_2$ predicted using the first-principles approach

Xiao-Wei Sun,\* Meng-Ru Chen, Ting Song, Jun-Hong Tian, Zi-Jiang Liu and Wen-Chao Huang

2638



### Anomalous Hall effect in Nd-doped $\text{Bi}_{1.1}\text{Sb}_{0.9}\text{STe}_2$ topological insulator single crystals

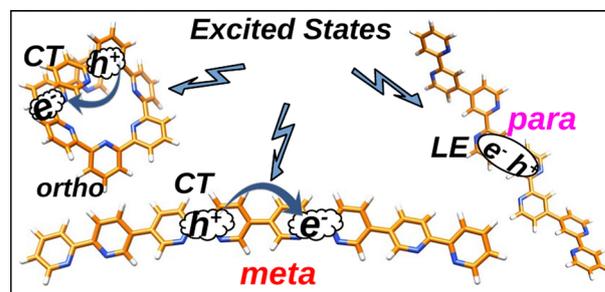
Lei Chen, Weiyao Zhao, Kaijian Xing, Mengyun You, Xiaolin Wang and Ren-Kui Zheng\*



2646

### Contrasting the excited state properties of different conformers of *trans*- and *cis*-2,2'-bipyridine oligomers in the gas phase

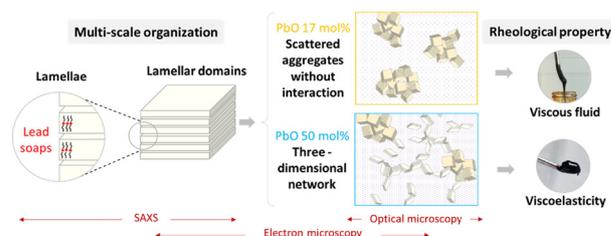
Palak Mandal and Aditya N. Panda\*



2657

### Multiscale organisation of lead carboxylates in artistic oil binders

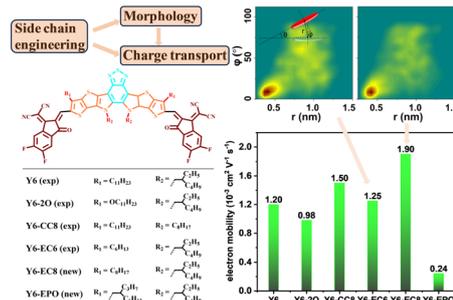
Lucie Laporte, Frédéric Gobeaux, Thierry Pouget, Nicolas Benoot, Julien Foison, David Touboul, Guylaine Ducouret and Laurence de Viguerie\*



2666

### The effects of side chain engineering on the morphology and charge transport of the A-DA<sub>1</sub>D-A type of non-fullerene acceptor: a multiscale study

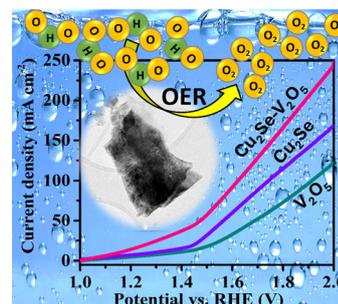
Zhijun Cao and Shaohui Zheng\*



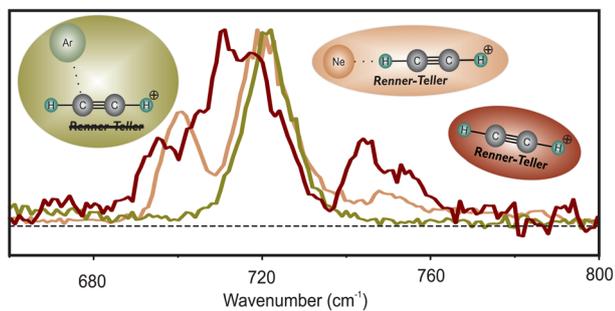
2678

### Synergistic effect of a bamboo-like Bi<sub>2</sub>S<sub>3</sub> covered Sm<sub>2</sub>O<sub>3</sub> nanocomposite (Bi<sub>2</sub>S<sub>3</sub>-Sm<sub>2</sub>O<sub>3</sub>) for enhanced alkaline OER

Tauseef Munawar, Saman Fatima, Khalid Mujasam Batoo, Ambreen Bashir, Faisal Mukhtar, Sajjad Hussain, Sumaira Manzoor, Muhammad Naeem Ashiq, Shoukat Alim Khan, Muammer Koc and Faisal Iqbal\*



2692



### Leak-out spectroscopy as alternative method to rare-gas tagging for the Renner–Teller perturbed $\text{HCCH}^+$ and $\text{DCCD}^+$ ions

Kim Steenbakkers, Tom van Boxtel,  
Gerrit C. Groenenboom, Oskar Asvany, Britta Redlich,  
Stephan Schlemmer and Sandra Brünken\*

