

## IN THIS ISSUE

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## COMMUNICATIONS

20168

### Regulation of stability and density of energetic materials via isomerism

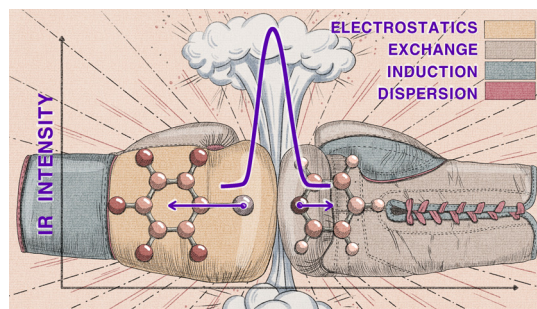
Wenjin Zhang, Yiling Yang, Shaoyi Shi, Siping Pang,  
Yuchuan Li\* and Chenghui Sun\*



20173

### Decoding the infrared spectra changes upon formation of molecular complexes: the case of halogen bonding in pyridine ··· perfluorohaloarene complexes

Alex Iglesias-Reguant, Heribert Reis, Miroslav Medved',  
Borys Ośmiatowski, Robert Zaleśny\* and Josep M. Luis\*



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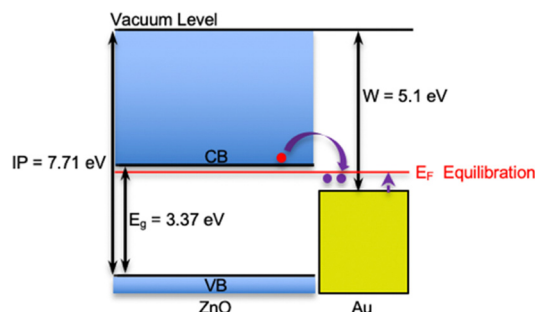


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**Fermi level shifts of gold nanospheres on ZnO film upon UV irradiation**

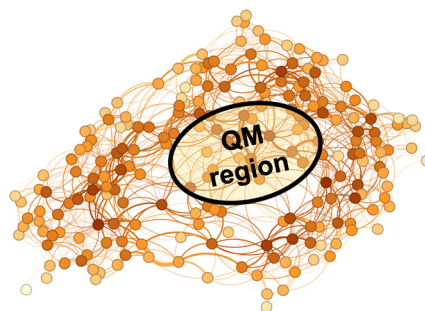
Grégory Barbillon



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**Protein network centralities as descriptor for QM region construction in QM/MM simulations of enzymes**

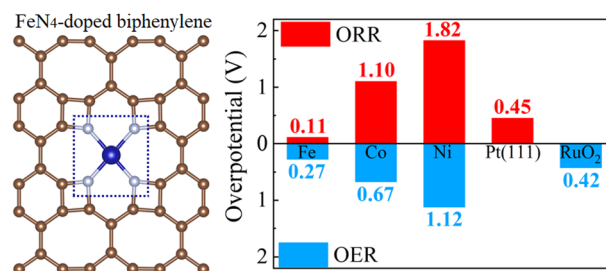
Felix Brandt and Christoph R. Jacob\*



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**Bifunctional electrocatalytic activity of Fe-embedded biphenylene for oxygen reduction and evolution reactions**

Junkai Xu, Yang Gao, Jing Li, Xun-Wang Yan\* and Fengjie Ma\*

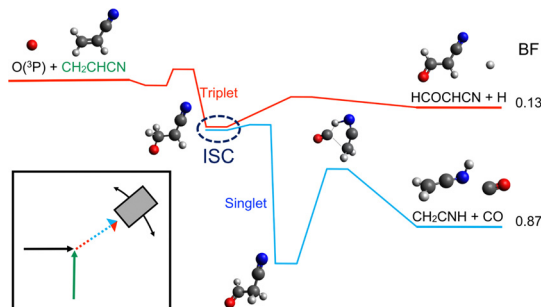


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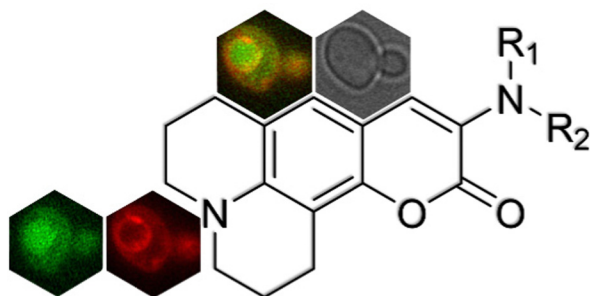
**A combined crossed molecular beam and theoretical study of the  $O(^3P, ^1D) + \text{acrylonitrile (CH}_2\text{CHCN)}$  reactions and implications for combustion and extraterrestrial environments**

Giacomo Pannacci, Luca Mancini, Gianmarco Vanuzzo, Pengxiao Liang, Demian Marchione, Marzio Rosi, Piergiorgio Casavecchia and Nadia Balucani\*



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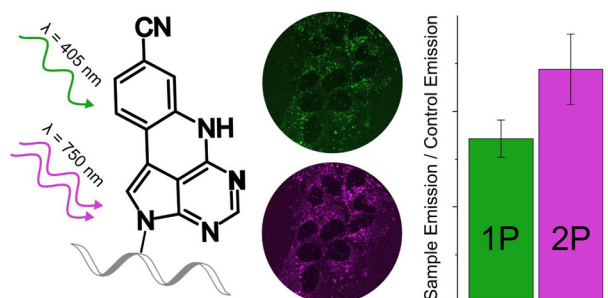
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### Rigidized 3-aminocoumarins as fluorescent probes for strongly acidic environments and rapid yeast vacuolar lumen staining: mechanism and application

Jakub Joniak, Henrieta Stankovičová, Šimon Budzák, Milan Sýkora, Katarína Gaplovská-Kyselá, Juraj Filo and Marek Cigáň\*

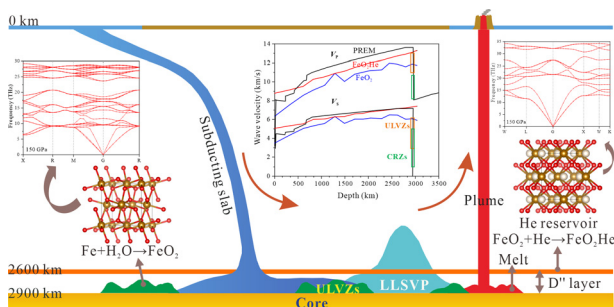
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### Multiphoton characterization and live cell imaging using fluorescent adenine analogue 2CNqA

Jesper R. Nilsson, Carlos Benitez-Martin, Henry G. Sansom, Pauline Pfeiffer, Tom Baladi, Hoang-Ngoan Le, Anders Dahlén, Steven W. Magennis and L. Marcus Wilhelmsson\*

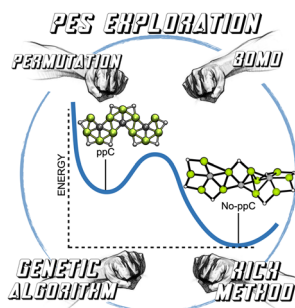
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### A first-principles study of the structural, electronic and elastic properties of the FeO<sub>2</sub>-FeO<sub>2</sub>He system under high pressure

Haibo Liu,\* Lei Liu,\* Cunlin Xin, Longxing Yang and Xiaoyu Gu

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### Revisiting the potential-energy surface of C<sub>n</sub>Be<sub>3n+2</sub>H<sub>2n+2</sub><sup>2+</sup> (*n* = 2–4) clusters: are planar pentacoordinate carbon structures the global minima?

Diego Inostroza, Alejandro Vásquez-Espinal, Luis Leyva-Parra, Williams García-Argote, María Luisa Cerón, Osvaldo Yañez and William Tiznado\*



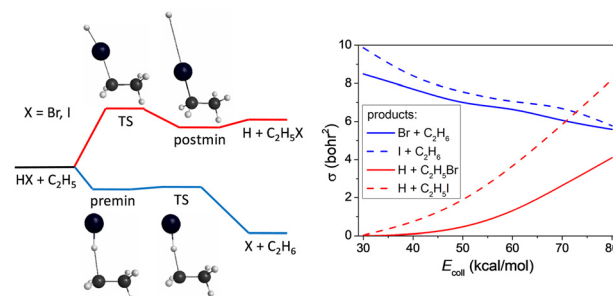


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# Competition between the H-abstraction and the X-abstraction pathways in the HX (X = Br, I) + C<sub>2</sub>H<sub>5</sub> reactions

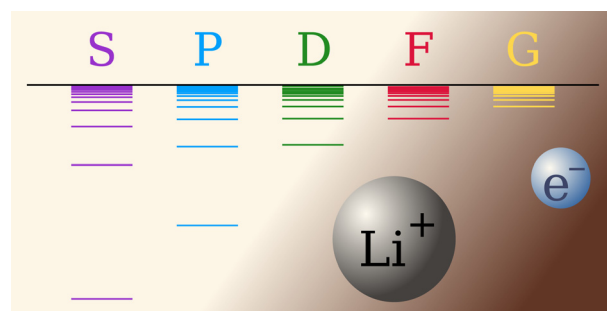
Cangtao Yin\* and Gábor Czakó\*



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# Using Koopmans' theorem for constructing basis sets: approaching high Rydberg excited states of lithium with a compact Gaussian basis

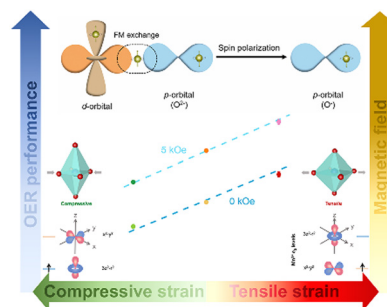
Jan Šmýdke



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# Enhanced oxygen evolution reaction via the tunability of spin polarization and electronic states in a flexible van der Waals membranous catalyst

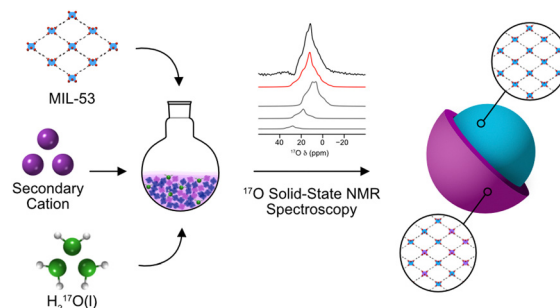
Hang Xu, Ji Qi, Yuan Zhang, Linglong Hu, Ming Feng\* and Weiming Lü\*



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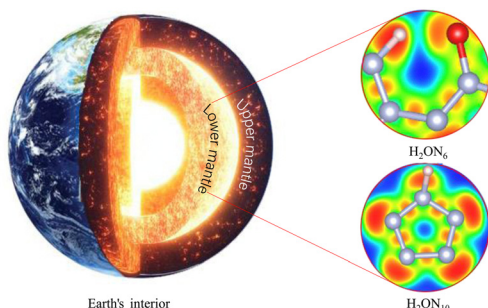
# Exploring cation distribution in ion-exchanged Al,Ga-containing metal-organic frameworks using <sup>17</sup>O NMR spectroscopy

Zachary H. Davis, Russell E. Morris\* and Sharon E. Ashbrook\*



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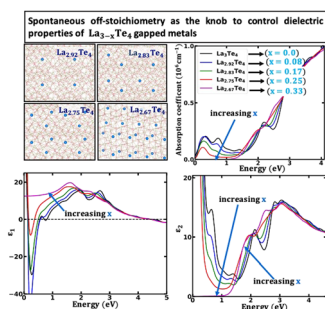
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### Prediction of a reservoir of N-rich high-energy density material at the Earth's mantle

Kang Yang, Jingming Shi,\* Wenwen Cui, Jian Hao and Yinwei Li\*

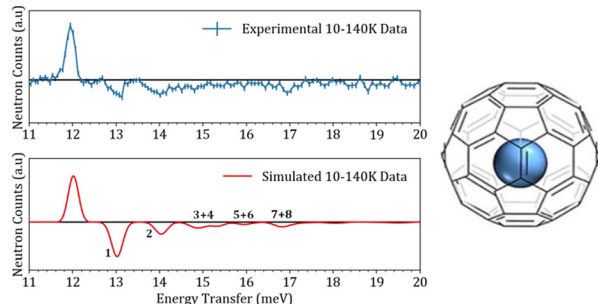
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### Spontaneous off-stoichiometry as the knob to control the dielectric properties of gapped metals

Muhammad Rizwan Khan, Harshan Reddy Gopidi, Hamid Reza Darabian, Dorota A. Pawlak and Oleksandr I. Malyi\*

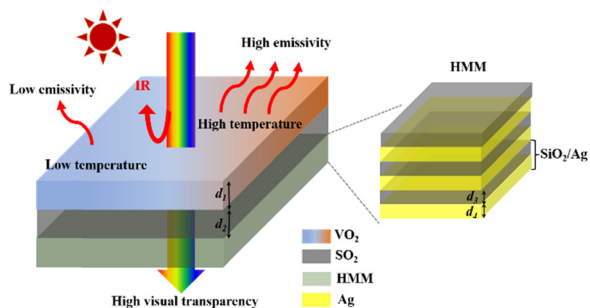
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### A combined inelastic neutron scattering and simulation study of the $^3\text{He}@C_{60}$ endofullerene

Mohamed Aouane, Jeff Armstrong, Mark Walkey, Gabriela Hoffman, George R. Bacanu, Richard J. Whitby, Malcolm H. Levitt and Stéphane Rols\*

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### Transparent spacecraft smart thermal control device based on $\text{VO}_2$ and hyperbolic metamaterials

Biyuan Wu, Derui Zhang, Cunhai Wang, Kaihua Zhang and Xiaohu Wu\*

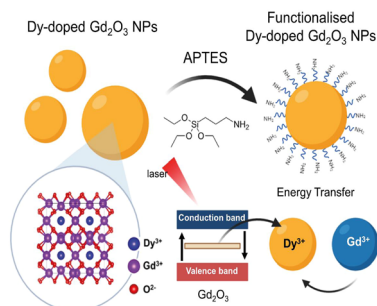


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**Structural and optical characterisation of silanised Dy-doped-Gd<sub>2</sub>O<sub>3</sub> NPs**

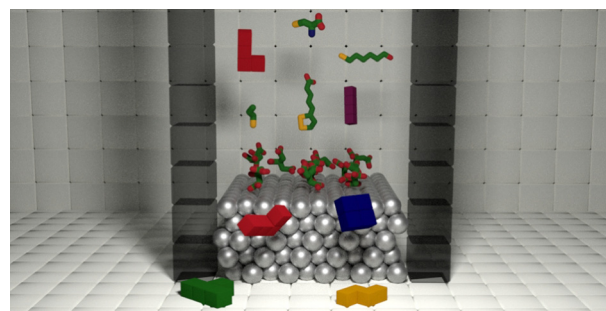
Erika Armenta-Jaime, Jorge Molina-González, Karla P. Salas-Martin, Raymond Fan, Lo-Yueh Chang, Jeng-Lung Chen, Paul Steadman, Haggeo Desirena-Enriquez, Ateet Dutt, Paul Olalde-Velasco\* and Silvia E. Castillo-Blum\*



20320

**Thermodynamics of the physisorption of capping agents on silver nanoparticles**

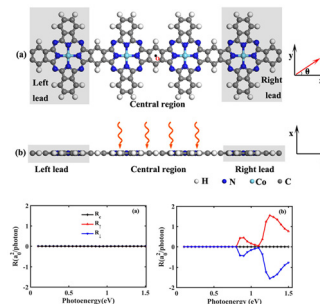
Matias Zúñiga-Bustos, Jeffrey Comer\* and Horacio Pobleto\*



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**Pure spin current in a cobalt phthalocyanine chain induced by the photogalvanic effect**

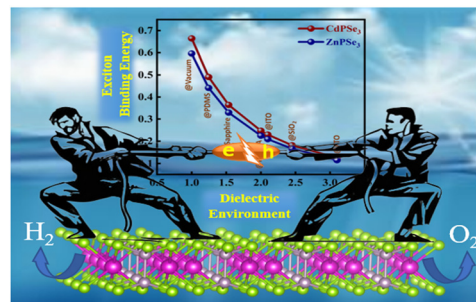
Xiaojie Liu, Bairui Tao, Yin Wang and Haitao Yin\*



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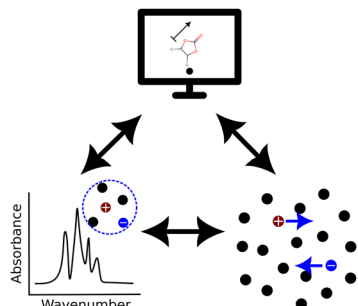
**Regulating excitonic effects in non-oxide based XPSe<sub>3</sub> (X = Cd, Zn) monolayers towards enhanced photocatalysis for overall water splitting**

Amal Kishore, Harshita Seksaria, Anu Arora and Abir De Sarkar\*



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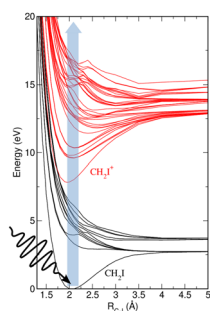
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### Mechanistic understanding of the correlation between structure and dynamics of liquid carbonate electrolytes: impact of polarization

Moumita Maiti, Anand Narayanan Krishnamoorthy, Youssef Mabrouk, Nataliia Mozhzhukhina, Aleksandar Matic, Diddo Diddens and Andreas Heuer\*

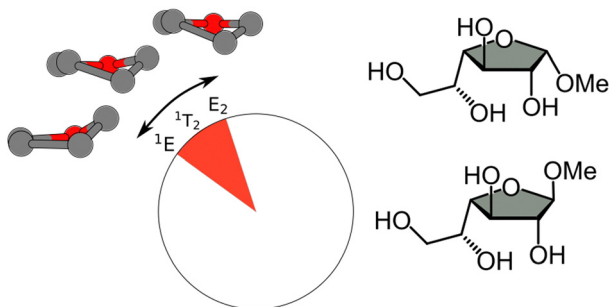
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### An *ab initio* study of the photodissociation of $\text{CH}_2\text{I}$ and $\text{CH}_2\text{I}^+$

A. Bouallagui, A. Zanchet, L. Bañares and A. Garcia-Vela\*

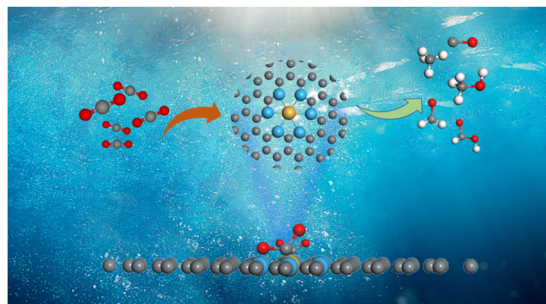
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### Conformational preferences of the flexible galactofuranose sugar in gas-phase

Oznur Yeni, Abdul-Rahman Allouche, Laurent Legentil, Vincent Ferrières and Isabelle Compagnon\*

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### Rare-earth metal- $\text{N}_6$ centers in porous carbon for electrocatalytic $\text{CO}_2$ reduction

Xianshi Zeng, Luliang Liao, Meishan Wang\* and Hongming Wang\*



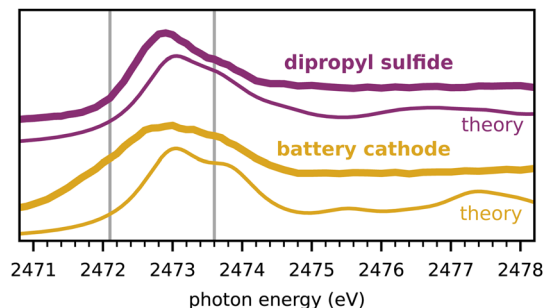


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### NEXAFS spectra of model sulfide chains: implications for sulfur networks obtained from inverse vulcanization

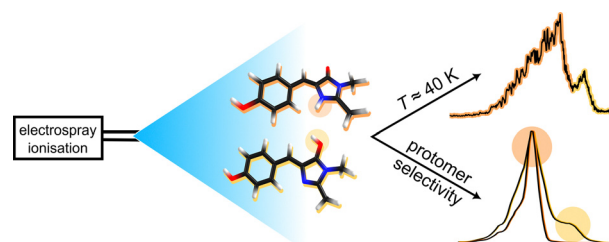
Sunel de Kock,\* Konstantin Skudler, Rukiya Matsidik, Michael Sommer, Matthias Müller and Michael Walter



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### Protomers of the green and cyan fluorescent protein chromophores investigated using action spectroscopy

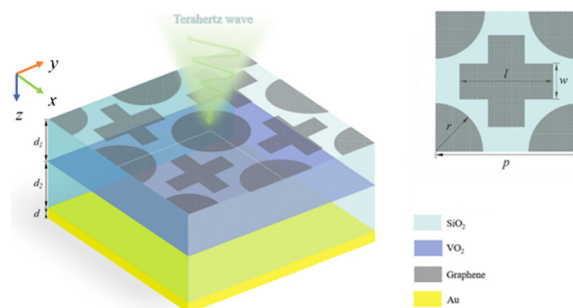
Eleanor K. Ashworth, Jordan Dezalay, Christopher R. M. Ryan, Christian Ieritano, W. Scott Hopkins, Isabelle Chambrier, Andrew N. Cammidge, Mark H. Stockett, Jennifer A. Noble and James N. Bull\*



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### A dual ultra-broadband switchable high-performance terahertz absorber based on hybrid graphene and vanadium dioxide

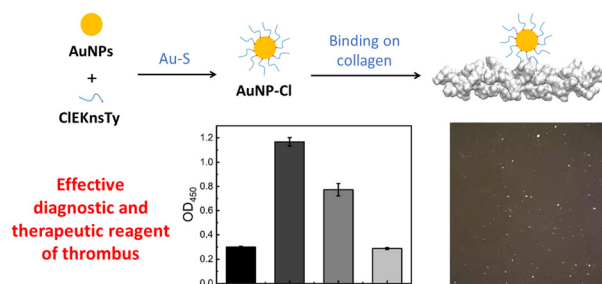
Wenya Chen, Chao Li,\* Dong Wang, Song Gao, Chunwei Zhang, Haijun Guo, Wei An, Shijing Guo and Guozheng Wu



20422

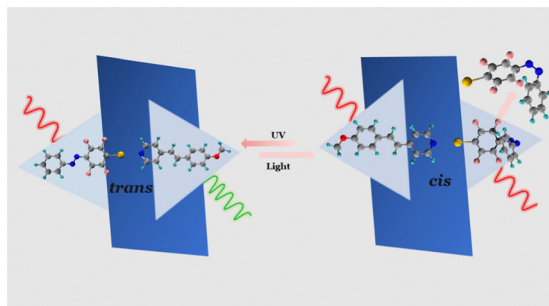
### Design and characterization of antithrombotic CIEKnsTy-Au nanoparticles as diagnostic and therapeutic reagents

Chen Xie and Lin Zhang\*



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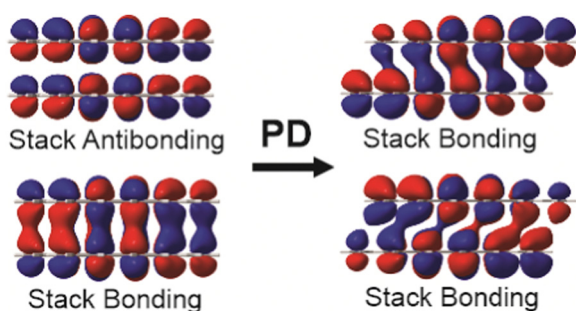
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### Photoswitchable nonlinear optical properties of azobenzene-based supramolecular complexes: insights from density functional theory

Aqsa Nisar, Sobia Tabassum, Khurshid Ayub, Tariq Mahmood, Hamad AlMohamadi, Asim Laeeq Khan, Muhammad Yasin, R. Nawaz and Mazhar Amjad Gilani\*

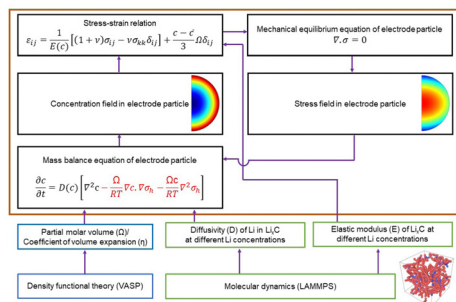
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### Stack bonding in polyaromatic hydrocarbons

Craig A. Bayse

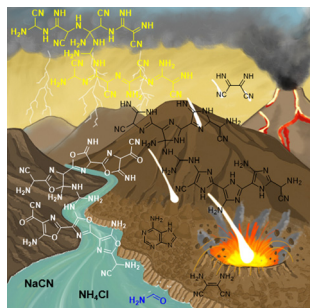
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### A comprehensive diffusion-induced stress coupled multiscale modeling and analysis in hard-carbon electrodes of Li-ion batteries

P. Pavan Kumar, Asutosh Agrawal, Debasis Nayak, Koushik Biswas, Sudipto Ghosh and Tarun Kumar Kundu\*

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### Ammonium affects the wet chemical network of HCN: feedback between prebiotic chemistry and materials science

Cristina Pérez-Fernández, Jorge Vega, José L. de la Fuente, Eva Mateo-Martí, Pilar Valles and Marta Ruiz-Bermejo\*

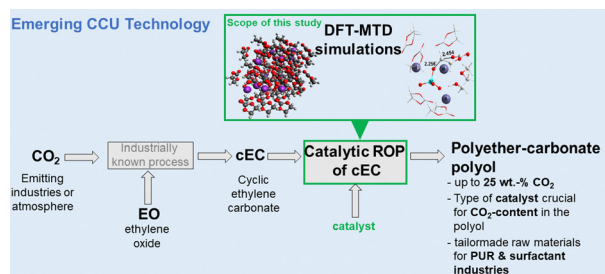


## RESEARCH PAPERS

20485

# A DFT-metadynamics study disclosing key properties of ring-opening polymerization catalysts to produce polyethercarbonate polyols from cyclic ethylene carbonate as part of an emerging CCU technology

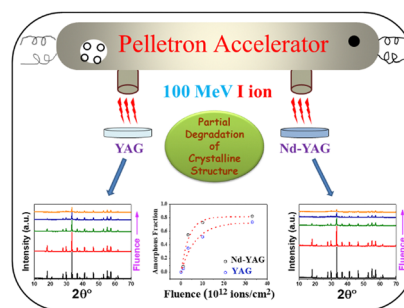
Mojgan Heshmat, Matthias Leven, Olga Linker, Marina Sebastian, Christoph Gürtler\* and Martin R. Machat\*



20495

# Radiation response of $\text{Y}_3\text{Al}_5\text{O}_{12}$ and $\text{Nd}^{3+}\text{-Y}_3\text{Al}_5\text{O}_{12}$ to Swift heavy ions: insight into structural damage and defect dynamics

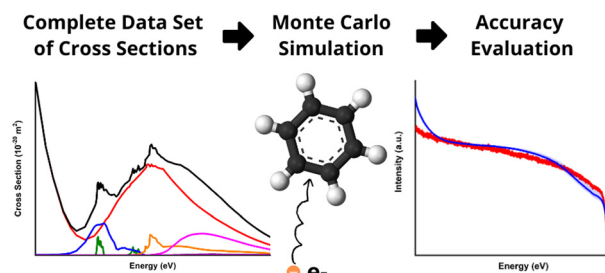
Koushik Bhandari, V. Grover,\* P. Kalita, K. Sudarshan, B. Modak, Saurabh K. Sharma and P. K. Kulriya



20510

# Evaluated electron scattering cross section dataset for gaseous benzene in the energy range 0.1–1000 eV

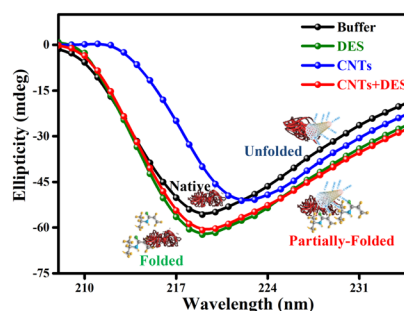
A. García-Abenza,\* A. I. Lozano,\* L. Álvarez, J. C. Oller, J. Rosado, F. Blanco, P. Limão-Vieira and G. García\*



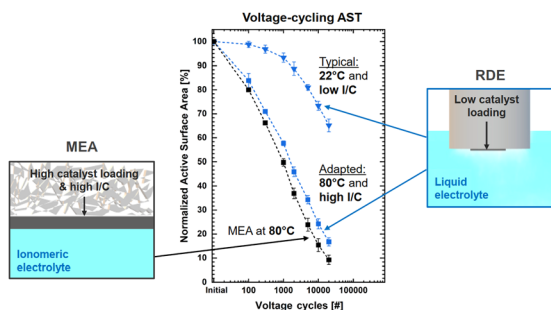
20519

# The attenuating ability of deep eutectic solvents towards the carboxylated multiwalled carbon nanotubes induced denatured $\beta$ -lactoglobulin structure

Niketa Yadav, Sanjay Mor and Pannuru Venkatesu\*



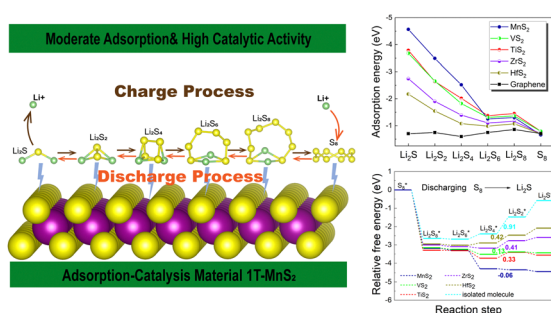
20533



### Towards a realistic prediction of catalyst durability from liquid half-cell tests

Timo Imhof,\* Roberta K. F. Della Bella, Björn M. Stühmeier, Hubert A. Gasteiger and Marc Ledendecker\*

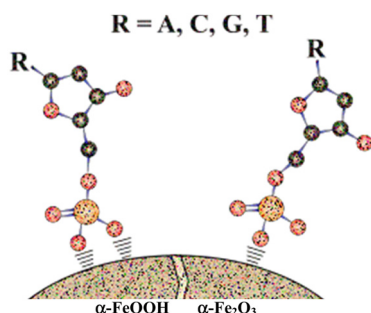
20546



### A computational study on bifunctional 1T-MnS<sub>2</sub> with an adsorption-catalysis effect for lithium–sulfur batteries

Shaorong Duan, Mingyi Liu, Chuanzhao Cao, Haitao Liu,\* Meng Ye\* and Wenhui Duan

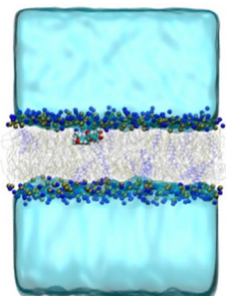
20557



### Distinguishing different surface interactions for nucleotides adsorbed onto hematite and goethite particle surfaces through ATR-FTIR spectroscopy and DFT calculations

Izaak Sit, Mark A. Young, James D. Kubicki\* and Vicki H. Grassian\*

20567



### Modelling the effects of *E/Z* photoisomerization of a cyclocurcumin analogue on the properties of cellular lipid membranes

Anastasiia Delova, Raul Losantos, Jérémy Pecourneau, Maxime Mourer, Andreea Pasc and Antonio Monari\*



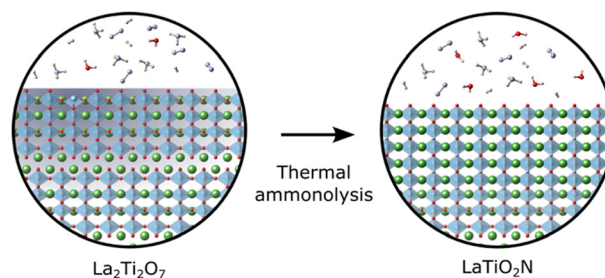


## RESEARCH PAPERS

20575

**Conversion of  $\text{La}_2\text{Ti}_2\text{O}_7$  to  $\text{LaTiO}_2\text{N}$  via ammonolysis: a first-principles investigation**

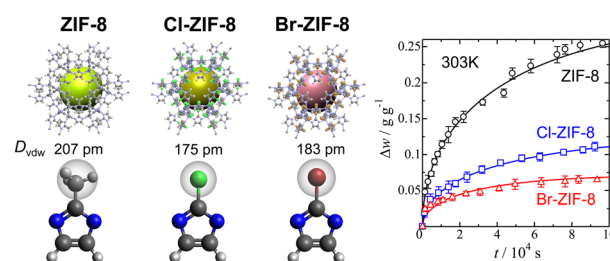
Chiara Ricca, Tristan Blandenier, Valérie Werner, Xing Wang, Simone Pokrant and Ulrich Aschauer\*



20585

**Substitution ( $\text{CH}_3$ , Cl, or Br) effects of the imidazolate linker on benzene adsorption kinetics for the zeolitic imidazolate framework (ZIF)-8**

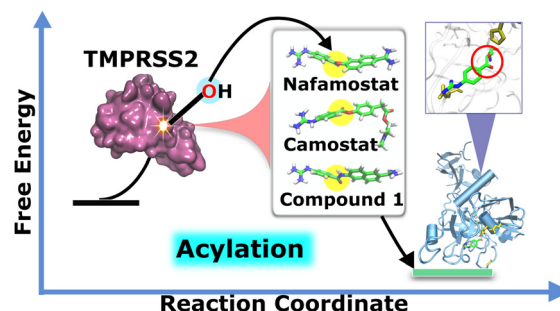
Ryohei Yagi and Takahiro Ueda\*



20597

**A quantum chemical study on the anti-SARS-CoV-2 activity of TMPRSS2 inhibitors**

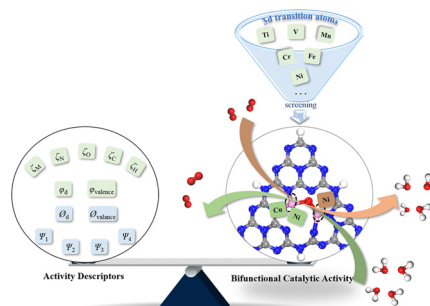
Akihiro Kondo, Kazuhiro J. Fujimoto\* and Takeshi Yanai\*



20606

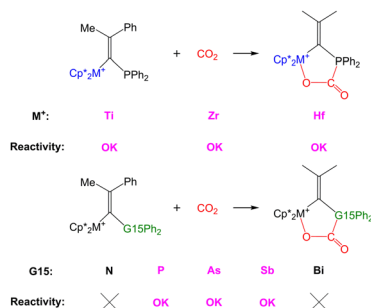
**Oxo transition metal anchored on  $\text{C}_3\text{N}_4$  with constructing a high-activity bifunctional electrocatalyst for rechargeable metal–air batteries**

Yahui Li, Xiuyun Zhao and Xin Chen\*



## RESEARCH PAPERS

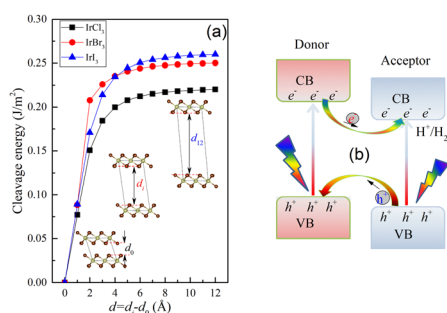
20618



### Computational insights into CO<sub>2</sub> binding reactions by intramolecular geminal group-IV<sup>+</sup>/phosphorus- and zirconium<sup>+</sup>/group-15-based frustrated Lewis pairs

Chi-Shiun Wu and Ming-Der Su\*

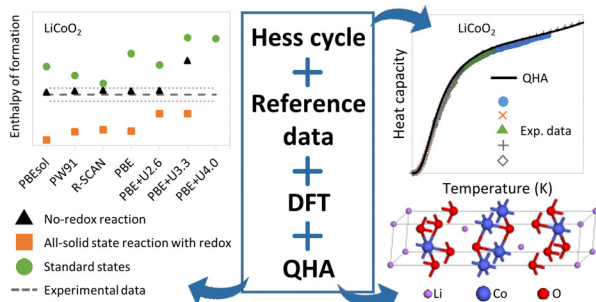
20632



### Stability and the electronic and optical properties of two-dimensional iridium trihalides with promising applications in photocatalytic water splitting

Ying-Xue Feng, Wen-Zhi Xiao,\* Qing-Yan Rong and Jiang-Lin Fang\*

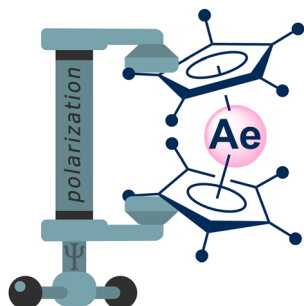
20641



### Thermodynamic properties of LiNiO<sub>2</sub>, LiCoO<sub>2</sub>, and LiMnO<sub>2</sub> using density-functional theory

Lucas Tosin Paese,\* Philippe Zeller, Sylvie Chatain and Christine Guéneau

20657



### Revisiting the origin of the bending in group 2 metallocenes AeCp<sub>2</sub> (Ae = Be–Ba)

Tetiana Sergeieva, T. Ilgin Demirer, Axel Wuttke, Ricardo A. Mata,\* André Schäfer,\* Gerrit-Jan Linker\* and Diego M. Andrada\*

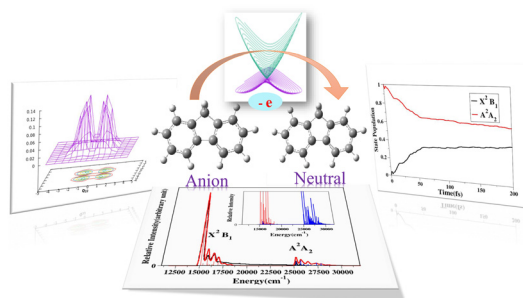


## RESEARCH PAPERS

20668

**Photodetachment band of the fluorenyl anion: a theoretical rationalization**

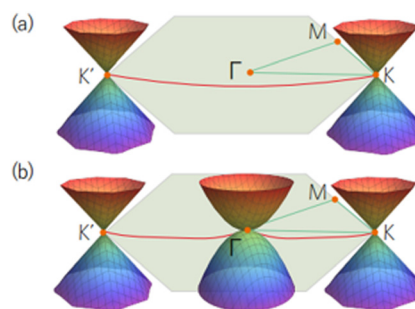
Abhishek Kumar, Preeti Karmakar, Rudraditya Sarkar\* and Tammineni Rajagopala Rao\*



20680

**Ideal topological Weyl complex phonons in two dimensions**

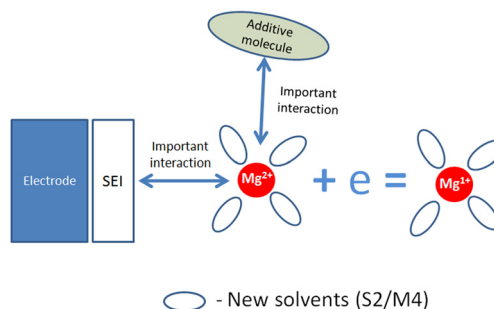
Wei-Wang Yu, Ying Liu,\* Zeqing He, Lirong Wang, Xiaoming Zhang and Guodong Liu\*



20686

**Effect of long range interactions on the reduction of divalent ions in *N,O*-chelating solvents**

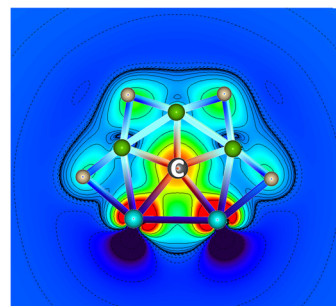
I. K. Bakulin and M. A. Orekhov\*



20693

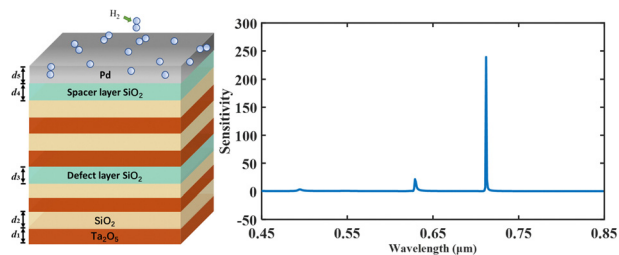
**Planar pentacoordinate carbon in a 16-electron neutral  $\text{CCu}_2\text{Be}_3\text{H}_4$  cluster**

Amlan J. Kalita, Namrata Gohain, Abhik Bordoloi and Ankur K. Guha\*



## RESEARCH PAPERS

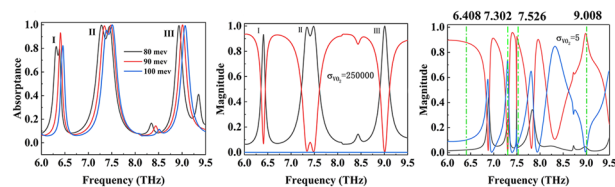
20697



### A dual-band hydrogen sensor based on Tamm plasmon polaritons

Kaihua Zhang, Zhiying Chen, Hongju Li, Zao Yi, Yufang Liu and Xiaohu Wu\*

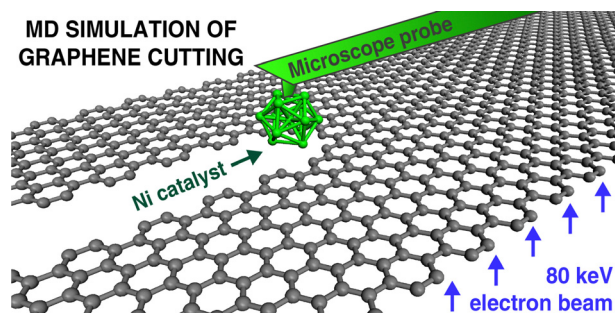
20706



### Dynamically changeable terahertz metamaterial absorbers with intelligent switch and high sensitivity and wide and narrow band perfect absorption

Qian Zhao, Zao Yi,\* Liang Bian, Huan Liu, Hua Yang, Shubo Cheng, Gongfa Li, Liangcai Zeng, Hailiang Li and Pinghui Wu

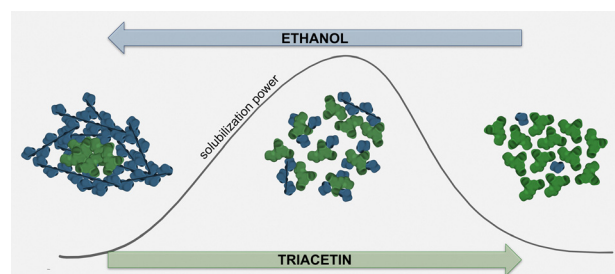
20715



### Precise graphene cutting using a catalyst at a probe tip under an electron beam

Alexander S. Sinitsa,\* Yulia G. Polinskaya, Irina V. Lebedeva, Andrey A. Knizhnik and Andrey M. Popov

20728



### In-depth study of binary ethanol–triacetin mixtures in relation to their excellent solubilization power

Evamaria Hofmann, Anna Saridis, Didier Touraud, Richard Buchner and Werner Kunz\*





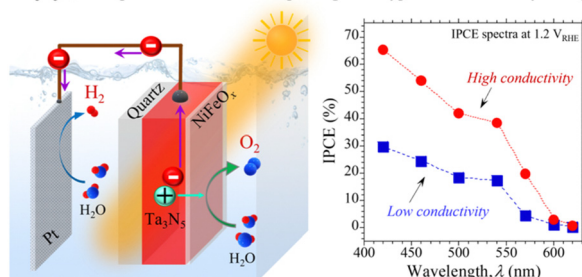
## RESEARCH PAPERS

20737

### Physicochemical insights into semiconductor properties of a semitransparent tantalum nitride photoanode for solar water splitting

Tomohiro Higashi,\* Hiroshi Nishiyama, Yuriy Pihosh, Kaisei Wakishima, Yudai Kawase, Yutaka Sasaki, Akira Nagaoka, Kenji Yoshino, Kazuhiro Takanabe and Kazunari Domen\*

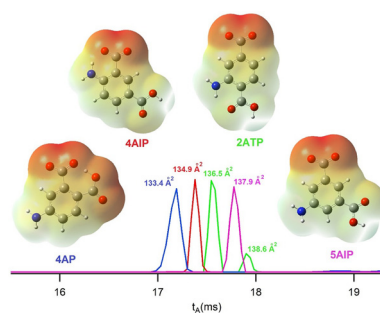
Ta<sub>3</sub>N<sub>5</sub>/Quartz photoanode for water splitting via n-type self-conductivity of Ta<sub>3</sub>N<sub>5</sub>



20749

### Mechanism of formation and ion mobility separation of protomers and deprotomers of diaminobenzoic acids and aminophthalic acids

Younes Valadbeigi\* and Tim Causon\*



## CORRECTIONS

20759

### Correction: Structure and bonding of molecular stirrers with formula B<sub>7</sub>M<sub>2</sub><sup>−</sup> and B<sub>8</sub>M<sub>2</sub> (M = Zn, Cd, Hg)

Rui Yu, Jorge Barroso, Meng-hui Wang, Wei-yan Liang, Chen Chen, Ximena Zarate, Mesias Orozco-Ic, Zhong-hua Cui\* and Gabriel Merino\*

20760

### Correction: A redshifted photonic bandgap and wide-angle polarization selection in an all-hyperbolic-metamaterial one-dimensional photonic crystal

Feng Wu,\* Dejun Liu, Hongju Li and Mingku Feng

