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COMMUNICATIONS

20168

Regulation of stability and density of energetic materials via isomerism

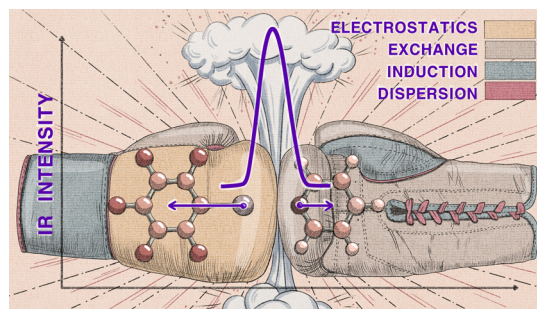
Wenjin Zhang, Yiling Yang, Shaoyi Shi, Siping Pang,
Yuchuan Li* and Chenghui Sun*



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 Ośmiałowski, Robert Zaleśny* and Josep M. Luis*



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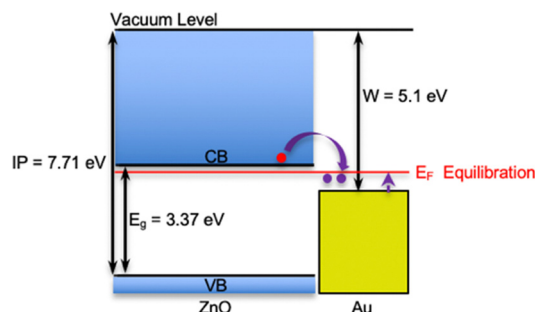


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20178

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

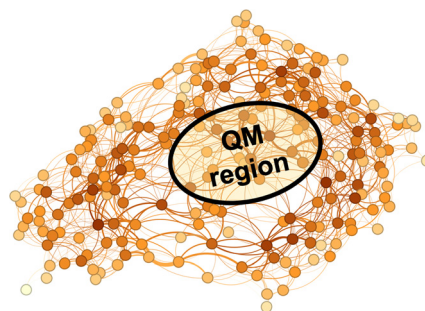
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20183

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

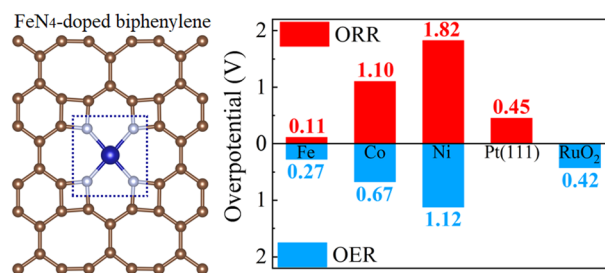
Felix Brandt and Christoph R. Jacob*



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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*

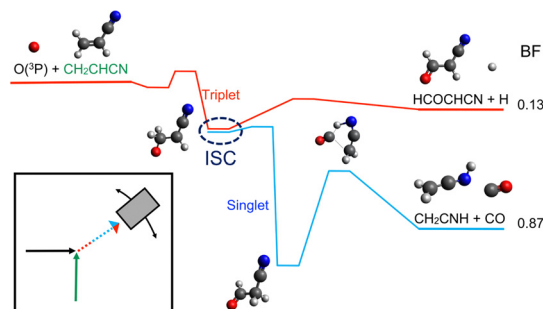


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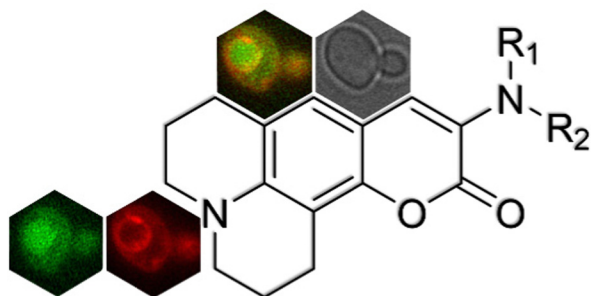
A combined crossed molecular beam and theoretical study of the O(³P, ¹D) + acrylonitrile (CH₂CHCN) reactions and implications for combustion and extraterrestrial environments

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



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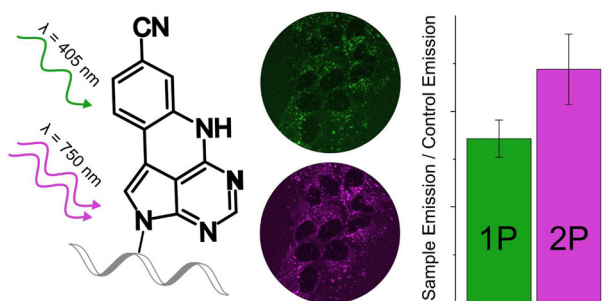
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Rigidized 3-aminocoumarins as fluorescent probes for strongly acidic environments and rapid yeast vacuolar lumen staining: mechanism and application

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

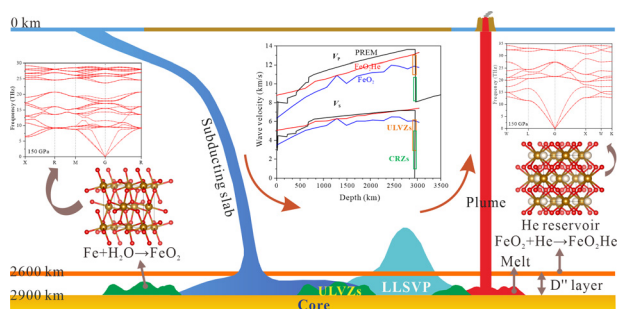
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Multiphoton characterization and live cell imaging using fluorescent adenine analogue 2CNqA

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*

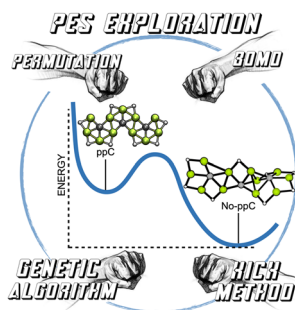
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A first-principles study of the structural, electronic and elastic properties of the $\text{FeO}_2\text{-FeO}_2\text{He}$ system under high pressure

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

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Revisiting the potential-energy surface of $\text{C}_n\text{Be}_{3n+2}\text{H}_{2n+2}^{2+}$ ($n = 2-4$) 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*

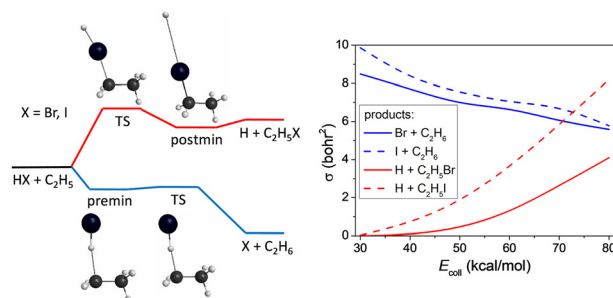


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Competition between the H-abstraction and the X-abstraction pathways in the HX (X = Br, I) + C₂H₅ reactions

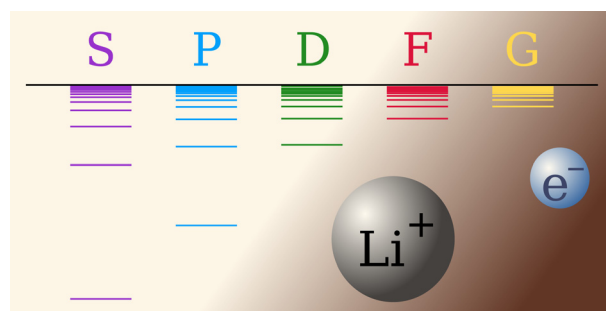
Cangtao Yin* and Gábor Czakó*



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

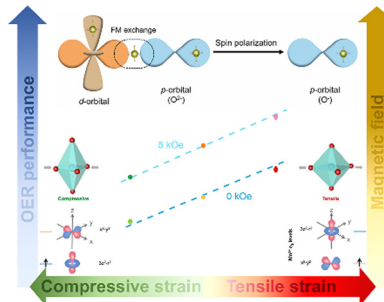
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Enhanced oxygen evolution reaction via the tunability of spin polarization and electronic states in a flexible van der Waals membranous catalyst

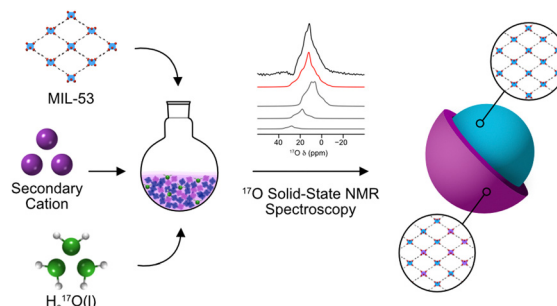
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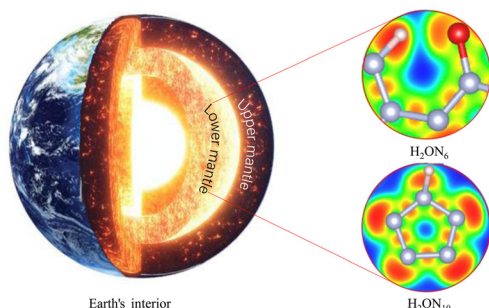
Exploring cation distribution in ion-exchanged Al,Ga-containing metal-organic frameworks using ¹⁷O NMR spectroscopy

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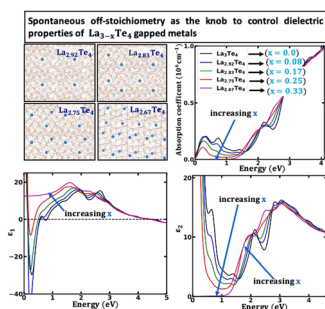
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Prediction of a reservoir of N-rich high-energy density material at the Earth's mantle

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

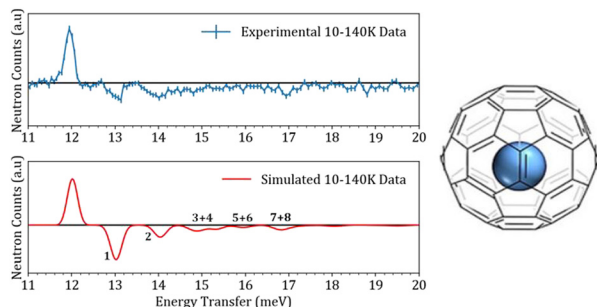
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Spontaneous off-stoichiometry as the knob to control the dielectric properties of gapped metals

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

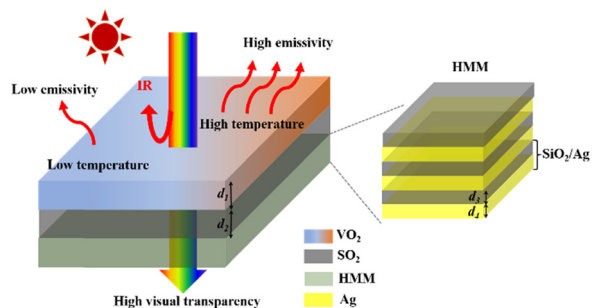
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A combined inelastic neutron scattering and simulation study of the $^3He@C_{60}$ endofullerene

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 VO_2 and hyperbolic metamaterials

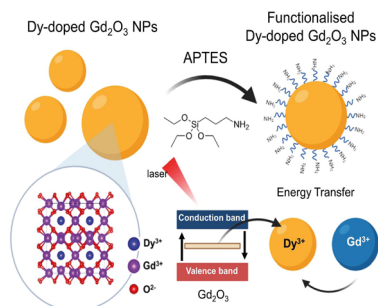
Biyuan Wu, Derui Zhang, Cunhai Wang, Kaihua Zhang and Xiaohu Wu*



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Structural and optical characterisation of silanised Dy-doped-Gd₂O₃ NPs

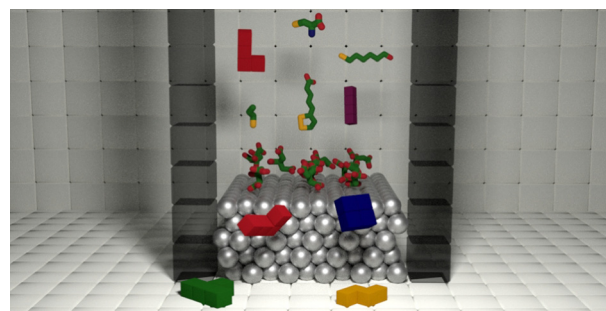
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20320

Thermodynamics of the physisorption of capping agents on silver nanoparticles

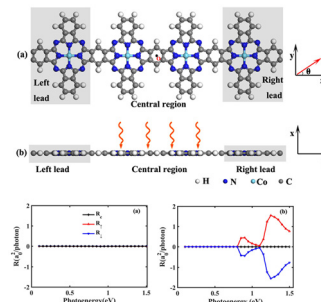
Matias Zúñiga-Bustos, Jeffrey Comer* and Horacio Pobleto*



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

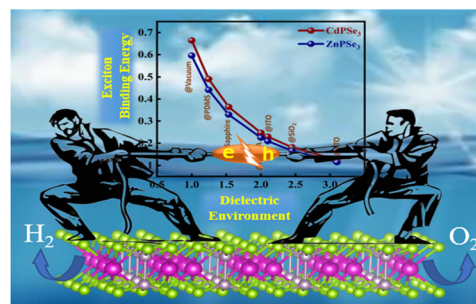
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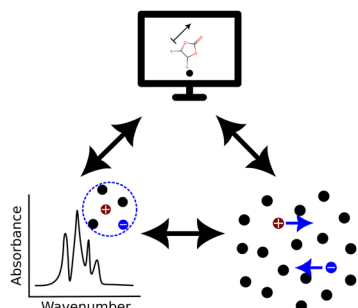
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Regulating excitonic effects in non-oxide based XPSe₃ (X = Cd, Zn) monolayers towards enhanced photocatalysis for overall water splitting

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



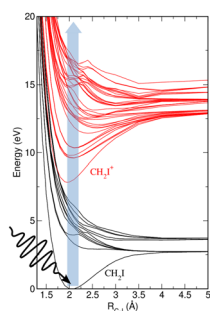
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Mechanistic understanding of the correlation between structure and dynamics of liquid carbonate electrolytes: impact of polarization

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

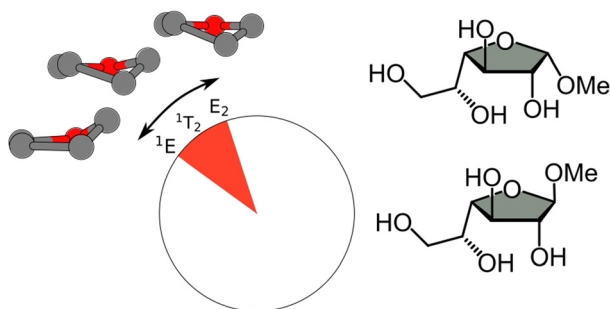
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An *ab initio* study of the photodissociation of CH_2I and CH_2I^+

A. Bouallagui, A. Zanchet, L. Bañares and A. García-Vela*

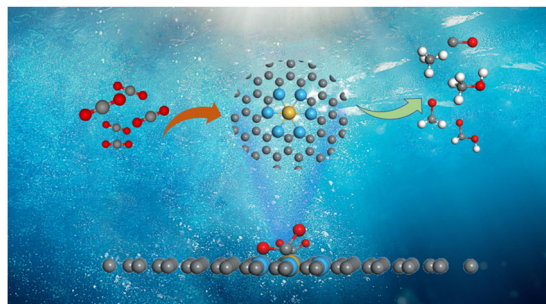
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Conformational preferences of the flexible galactofuranose sugar in gas-phase

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

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Rare-earth metal- N_6 centers in porous carbon for electrocatalytic CO_2 reduction

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

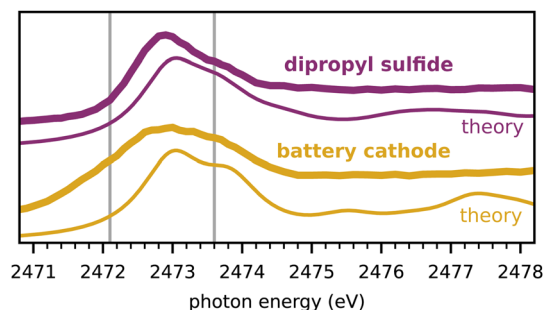


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NEXAFS spectra of model sulfide chains: implications for sulfur networks obtained from inverse vulcanization

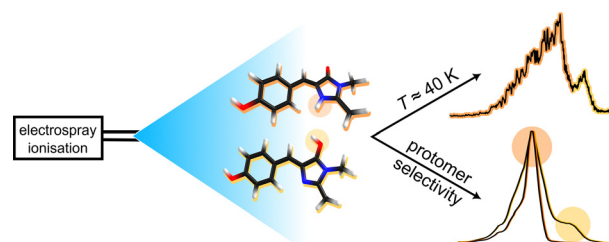
Sunel de Kock,* Konstantin Skudler, Rukiya Matsidik, Michael Sommer, Matthias Müller and Michael Walter



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

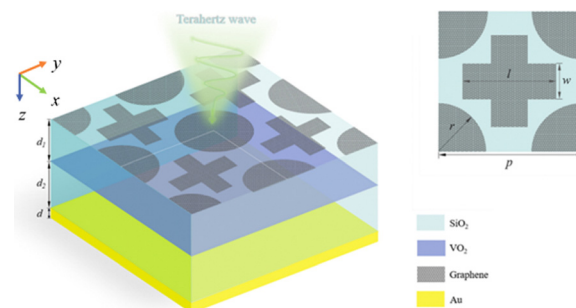
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20414

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

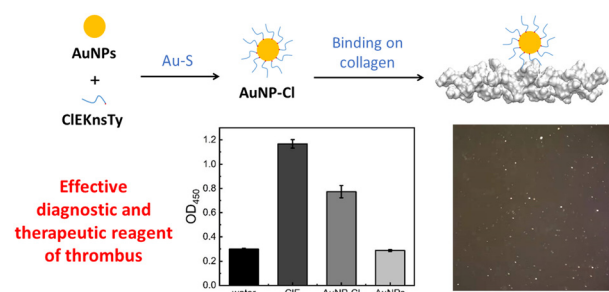
Wenya Chen, Chao Li,* Dong Wang, Song Gao, Chunwei Zhang, Haijun Guo, Wei An, Shijing Guo and Guozheng Wu



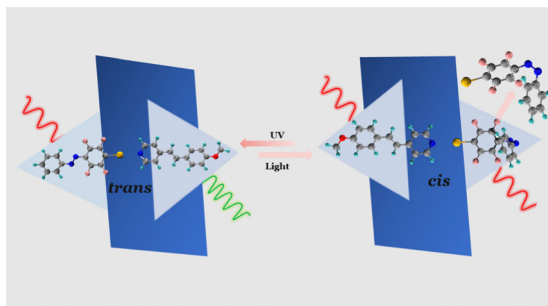
20422

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

Chen Xie and Lin Zhang*



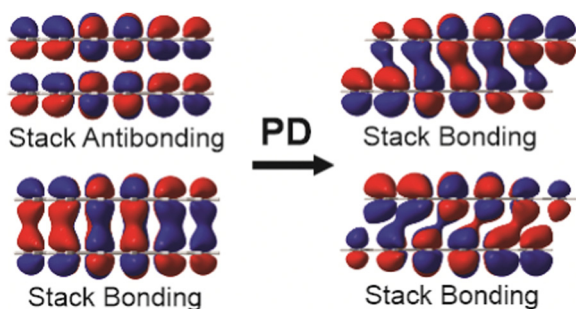
20430



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*

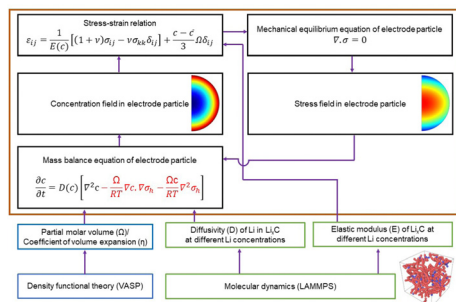
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Stack bonding in polyaromatic hydrocarbons

Craig A. Bayse

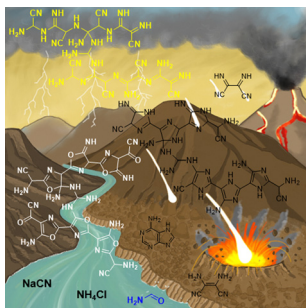
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A comprehensive diffusion-induced stress coupled multiscale modeling and analysis in hard-carbon electrodes of Li-ion batteries

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*

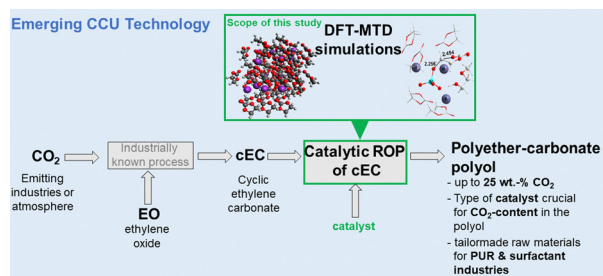


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A DFT-metadynamics study disclosing key properties of ring-opening polymerization catalysts to produce polyethercarbonate polyols from cyclic ethylene carbonate as part of an emerging CCU technology

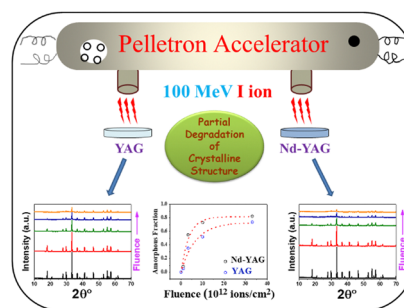
Mojgan Heshmat, Matthias Leven, Olga Linker, Marina Sebastian, Christoph Gürtler* and Martin R. Machat*



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Radiation response of $Y_3Al_5O_{12}$ and $Nd^{3+}-Y_3Al_5O_{12}$ to Swift heavy ions: insight into structural damage and defect dynamics

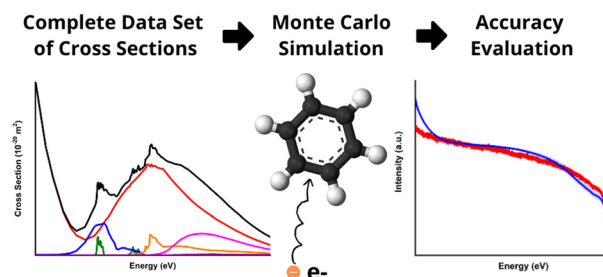
Koushik Bhandari, V. Grover,* P. Kalita, K. Sudarshan, B. Modak, Saurabh K. Sharma and P. K. Kulriya



20510

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

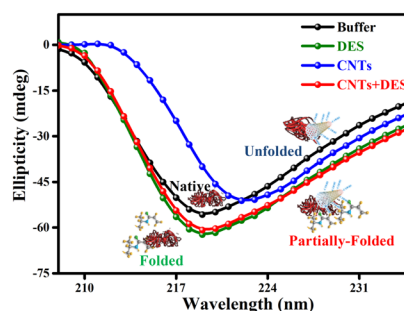
A. García-Abenza,* A. I. Lozano,* L. Álvarez, J. C. Oller, J. Rosado, F. Blanco, P. Limão-Vieira and G. García*



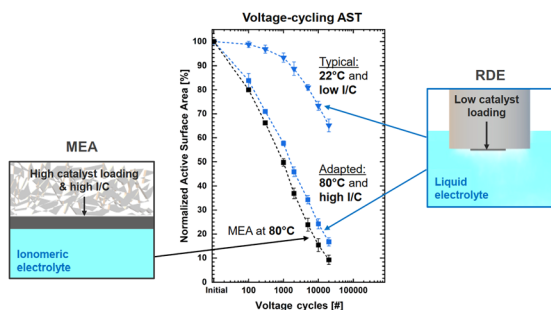
20519

The attenuating ability of deep eutectic solvents towards the carboxylated multiwalled carbon nanotubes induced denatured β -lactoglobulin structure

Niketa Yadav, Sanjay Mor and Pannuru Venkatesu*



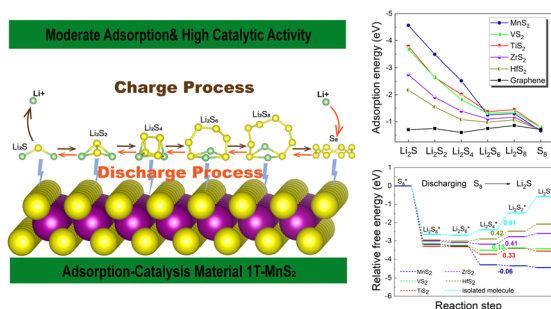
20533



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*

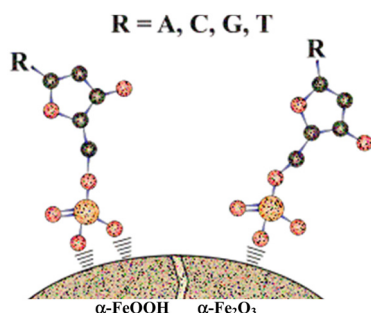
20546



A computational study on bifunctional 1T-MnS₂ with an adsorption-catalysis effect for lithium-sulfur batteries

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

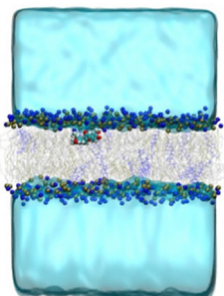
20557



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*

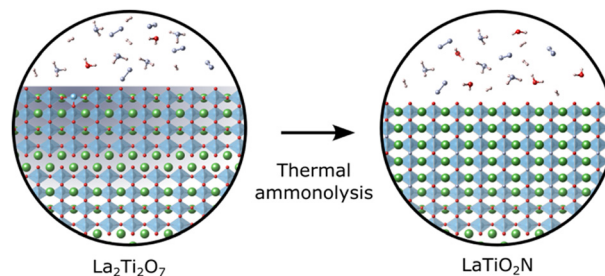


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20575

Conversion of $\text{La}_2\text{Ti}_2\text{O}_7$ to LaTiO_2N via ammonolysis: a first-principles investigation

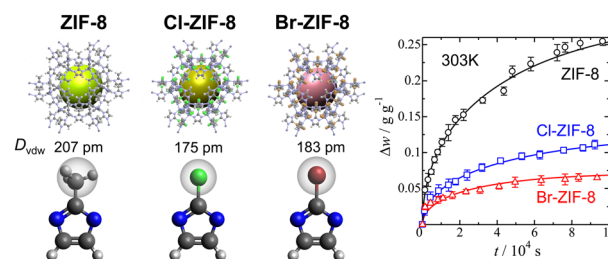
Chiara Ricca, Tristan Blandenier, Valérie Werner, Xing Wang, Simone Pokrant and Ulrich Aschauer*



20585

Substitution (CH_3 , Cl, or Br) effects of the imidazolate linker on benzene adsorption kinetics for the zeolitic imidazolate framework (ZIF)-8

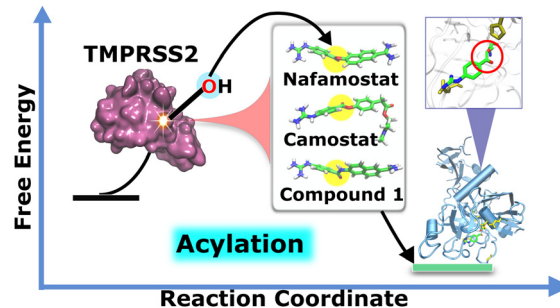
Ryohei Yagi and Takahiro Ueda*



20597

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

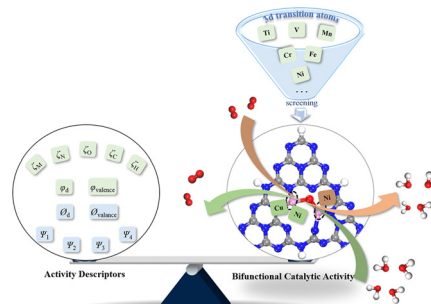
Akihiro Kondo, Kazuhiro J. Fujimoto* and Takeshi Yanai*



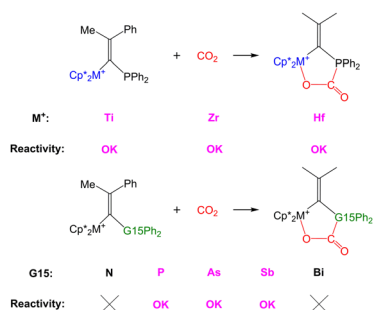
20606

Oxo transition metal anchored on C_3N_4 with constructing a high-activity bifunctional electrocatalyst for rechargeable metal–air batteries

Yahui Li, Xiuyun Zhao and Xin Chen*



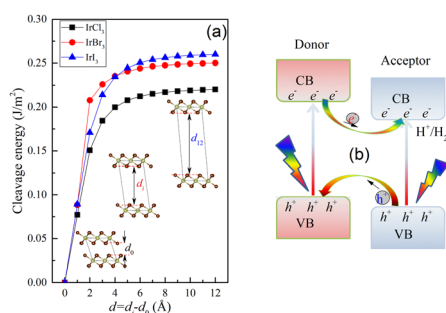
20618



Computational insights into CO₂ binding reactions by intramolecular geminal group-IV⁺/phosphorus- and zirconium⁺/group-15-based frustrated Lewis pairs

Chi-Shiun Wu and Ming-Der Su*

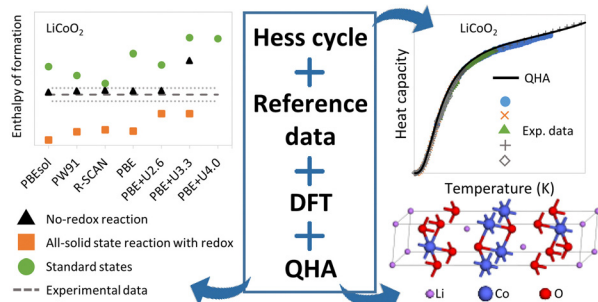
20632



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*

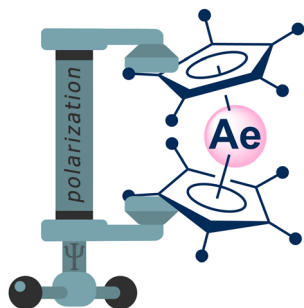
20641



Thermodynamic properties of LiNiO₂, LiCoO₂, and LiMnO₂ 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 AeCp₂ (Ae = Be–Ba)

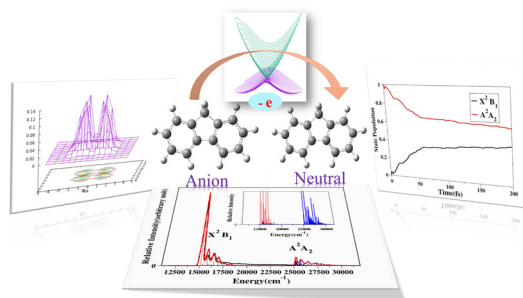
Tetiana Sergeieva, T. Ilgin Demirer, Axel Wuttke, Ricardo A. Mata,* André Schäfer,* Gerrit-Jan Linker* and Diego M. Andrada*



20668

Photodetachment band of the fluorenyl anion: a theoretical rationalization

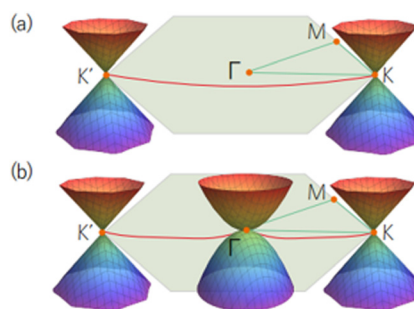
Abhishek Kumar, Preeti Karmakar, Rudraditya Sarkar* and Tammineni Rajagopala Rao*



20680

Ideal topological Weyl complex phonons in two dimensions

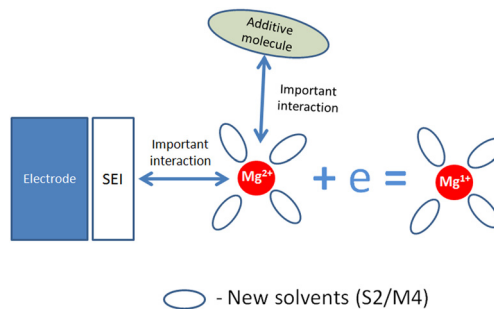
Wei-Wang Yu, Ying Liu,* Zeqing He, Lirong Wang, Xiaoming Zhang and Guodong Liu*



20686

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

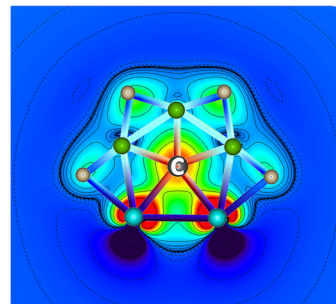
I. K. Bakulin and M. A. Orekhov*



20693

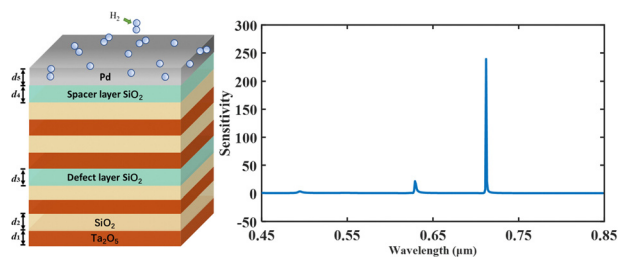
Planar pentacoordinate carbon in a 16-electron neutral $\text{CCu}_2\text{Be}_3\text{H}_4$ cluster

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



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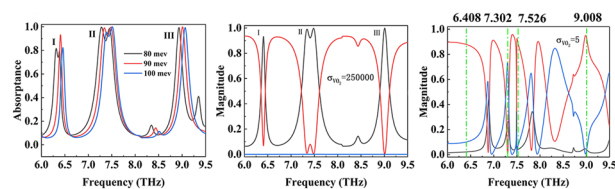
20697



A dual-band hydrogen sensor based on Tamm plasmon polaritons

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

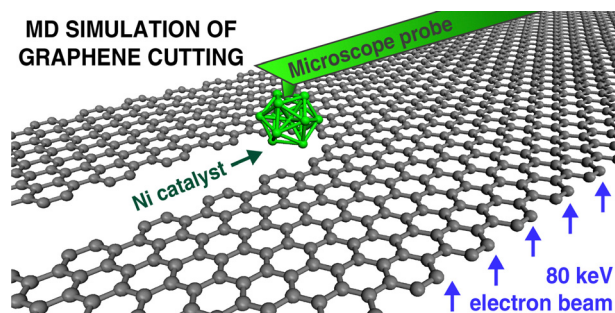
20706



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

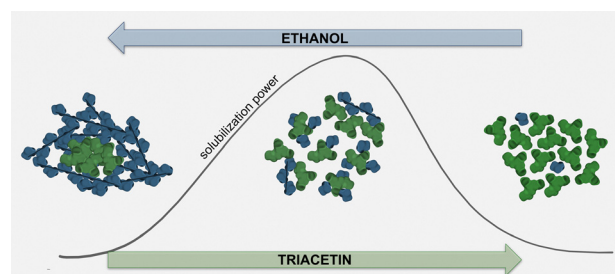
20715



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

Alexander S. Sinitsa,* Yulia G. Polynskaya, 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*



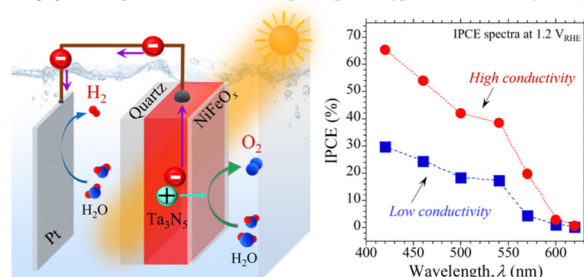
RESEARCH PAPERS

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*

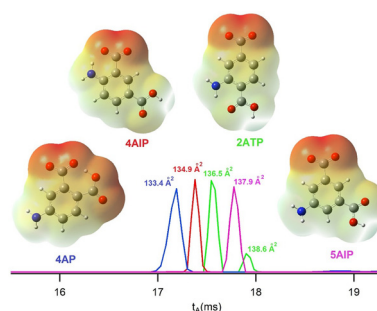
Ta₃N₅/Quartz photoanode for water splitting via n-type self-conductivity of Ta₃N₅



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 B₇M₂⁻ and B₈M₂ (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

