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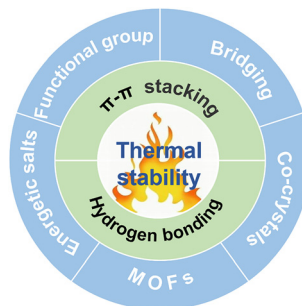
See Dennis Tokaryk, Stephen Ross *et al.*, pp. 18659–18678. Image reproduced by permission of Stephen Ross from *Phys. Chem. Chem. Phys.*, 2023, 25, 18659. Background image credit: Canadian Light Source Inc.

REVIEWS

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Thermal stability of azole-rich energetic compounds: their structure, density, enthalpy of formation and energetic properties

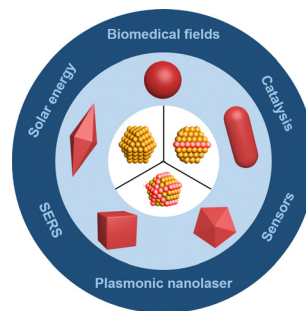
Xiangyan Miao, Xinbo Yang, Yuchuan Li* and Siping Pang*



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Recent progress of gold nanostructures and their applications

Khadiga Ali Dahan, Ying Li, Juan Xu* and Caixia Kan*



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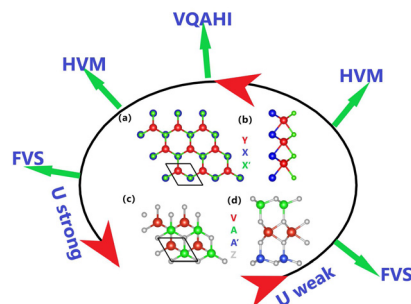


REVIEWS

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Correlation-driven topological phase transition in 2D valleytronic materials: a mini-review

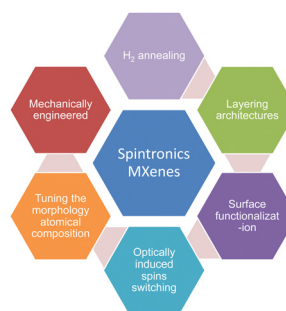
Xiao-Shu Guo and San-Dong Guo*



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Potential of MXenes as a novel material for spintronic devices: a review

Tahta Amrillah,* Angga Hermawan, Yerima Budi Cristian, Agustina Oktafiani, Diva Meisya Maulina Dewi, Ilma Amalina, Darminto and Jenh-Yih Juang

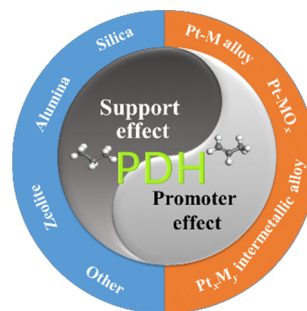


PERSPECTIVES

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Recent progress in catalytic dehydrogenation of propane over Pt-based catalysts

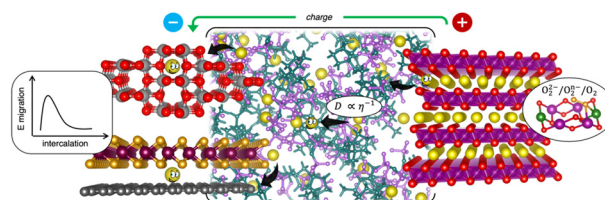
Yiou Shan, Huimin Hu, Xiaoqiang Fan* and Zhen Zhao*



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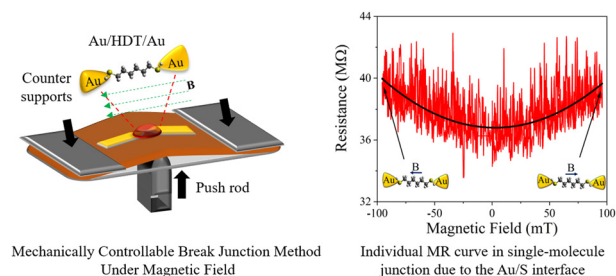
First-principles design of nanostructured electrode materials for Na-ion batteries: challenges and perspectives

Arianna Massaro,* Francesca Fasulo, Adriana Pecoraro, Aniello Langella, Ana B. Muñoz-García and Michele Pavone*



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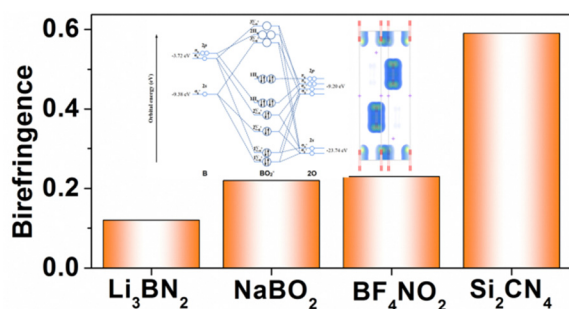
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Magnetoresistance originated from the Au/S interface in Au/1,6-hexanedithiol/Au single-molecule junctions at room temperature

Rachmat Andika, Ryo Yamada and Hirokazu Tada*

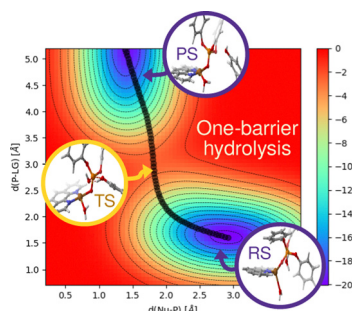
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Linear π -conjugated units of the $D_{\infty h}$ point group as superior ultraviolet birefringent units

Rong Yang, Abudukadi Tudi,* Yu Dang, Kewang Zhang and Hongsheng Shi*

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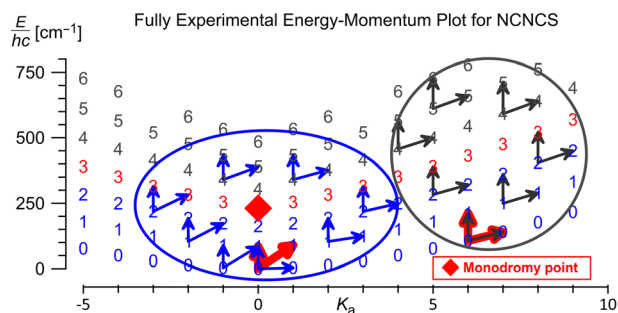


Hydrolysis of ester phosphates mediated by a copper complex

Brandon Meza-González and Fernando Cortés-Guzmán*

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Quantum monodromy in NCNCS – direct experimental confirmation

Dennis W. Tokaryk,* Stephen C. Ross, Manfred Winnewisser, Brenda P. Winnewisser, Frank C. De Lucia and Brant E. Billinghurst

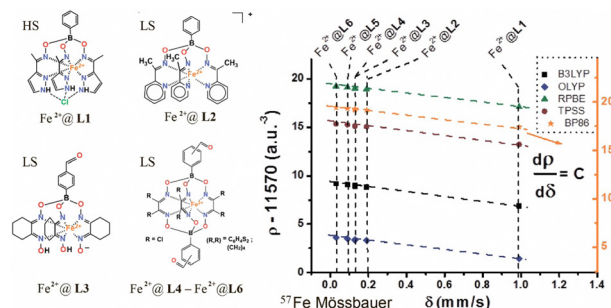


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 ^{57}Fe Mössbauer and DFT study of the electronic and spatial structures of the iron(II) (pseudo)clathrochelates: the effect of ligand field strength

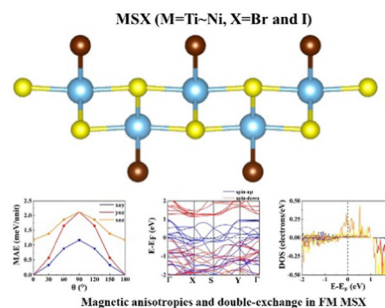
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Mechanical, magnetic and electronic properties of 2D MSX ($M = \text{Ti, V, Co and Ni, X = Br and I}$)

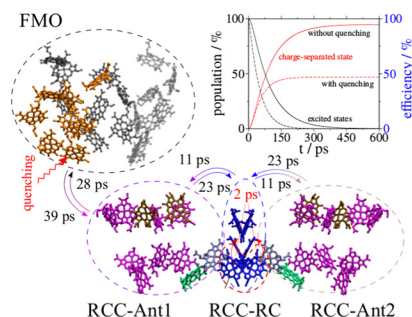
Yutong Li, Bowen Li, Haoyun Bai, Zhichao Yu, Chi Tat Kwok* and Hui Pan*



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Living on the edge: light-harvesting efficiency and photoprotection in the core of green sulfur bacteria

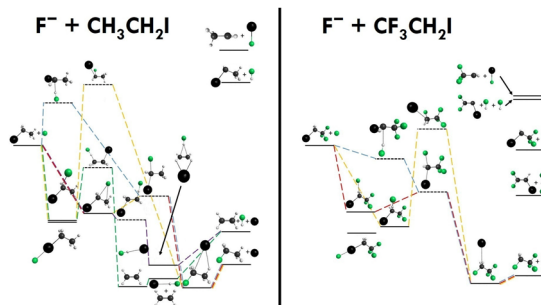
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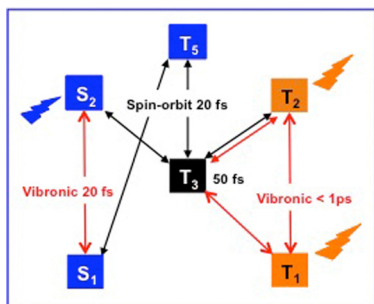
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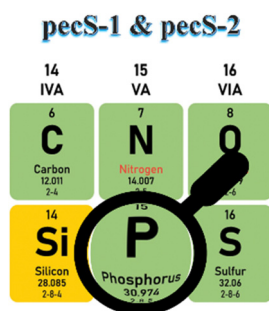
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Spin–vibronic mechanism at work in a luminescent square-planar cyclometalated tridentate Pt(II) complex: absorption and ultrafast photophysics

Souvik Mandal and Chantal Daniel*

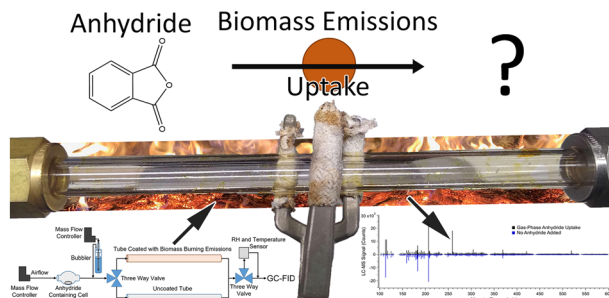
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New efficient pecS-*n* (*n* = 1, 2) basis sets for quantum chemical calculations of ³¹P NMR chemical shifts

Yuriy Yu. Rusakov and Irina L. Rusakova*

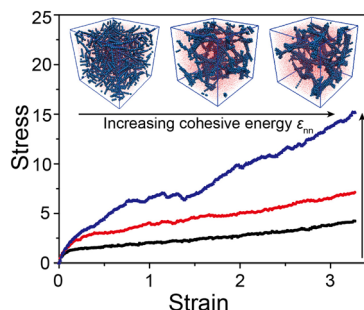
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Unexpected electrophiles in the atmosphere – anhydride nucleophile reactions and uptake to biomass burning emissions

Max Loebel Roson, Maya Abou-Ghanem, Erica Kim, Shuang Wu, Dylan Long, Sarah A. Styler and Ran Zhao*

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Revealing the reinforcing effect of a nanorod network on a polymer matrix through molecular dynamics simulations

Xiu Li, Ben Huang, Jun Liu,* Xiaoxi Hu and Zi-Jian Zheng*

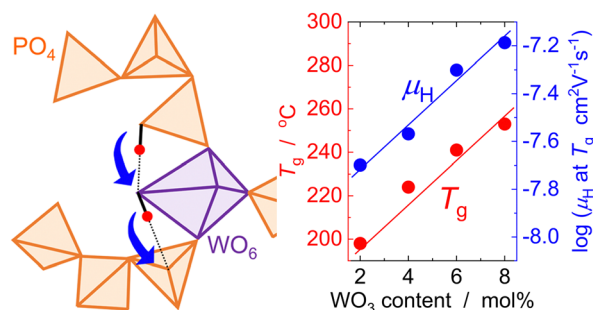


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Enhancing proton mobility and thermal stability in phosphate glasses with WO_3 : the mixed glass former effect in proton conducting glasses

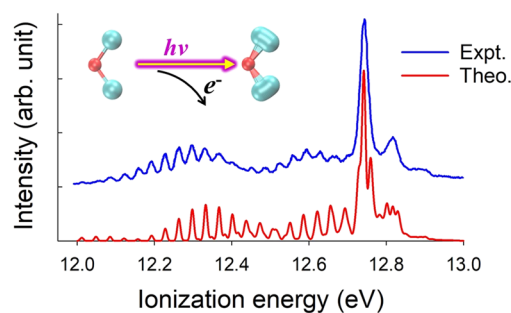
Aman Sharma, Issei Suzuki, Tomohiro Ishiyama and Takahisa Omata*



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Simulating the HeI photoelectron spectrum of Cl_2O with new full-dimensional adiabatic potential energy surfaces of $\text{Cl}_2\text{O}(\tilde{X}^1\text{A}_1)$, $\text{Cl}_2\text{O}^+(\tilde{X}^2\text{B}_1)$, and $\text{Cl}_2\text{O}^+(\tilde{C}^2\text{A}_2)$ and a three-state diabatic potential energy matrix of $\text{Cl}_2\text{O}^+(\tilde{A}^2\text{B}_2, \tilde{B}^2\text{A}_1, \text{and } 2^2\text{A}_1)$: a quantum mechanical study

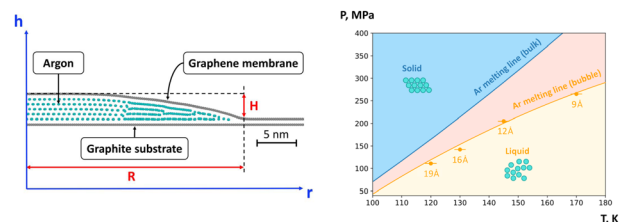
Zhe Hou, Siting Hou, Changjian Xie* and Huixian Han*



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Solid–liquid phase transition inside van der Waals nanobubbles: an atomistic perspective

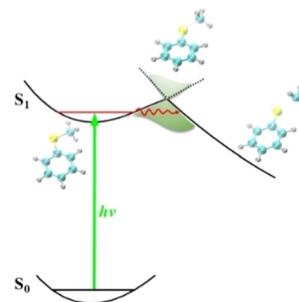
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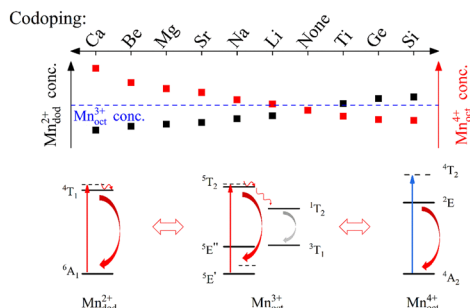
Nonadiabatic heavy atom tunneling in $^1\text{n}\sigma^*$ -mediated photodissociation of thioanisole

Chaofan Li, Siting Hou, Zhimo Wang and Changjian Xie*



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Mechanistic insights for regulating the site occupancy, valence states and optical transitions of Mn ions in yttrium–aluminum garnets *via* codoping

Qiaoling Chen, Mingzhe Liu, Chong-Geng Ma and Chang-Kui Duan*

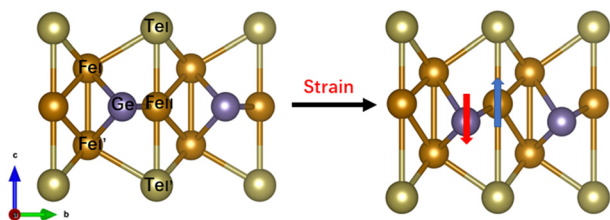
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Investigation of thermal control in phase-changing ABO₃ perovskites *via* first-principles predictions: general mechanism of solar absorptivity

Liping Tong, Hongchao Li, Hao Gong, Nianao Xu, Zhongyang Wang,* Qixin Guo and Tongxiang Fan*

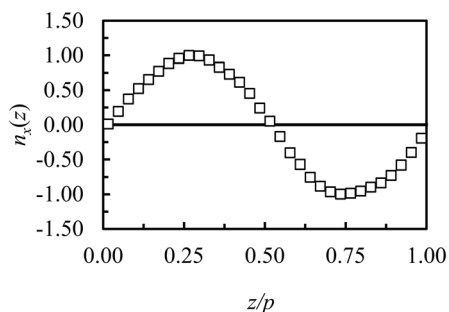
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A strain induced polar metal phase in a ferromagnetic Fe₃GeTe₂ monolayer

Xiaoyan Miao, Si Li, Zhenyi Jiang, Chunmei Zhang* and Aijun Du

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Diffusion-driven rotation in cholesteric liquid crystals studied using molecular dynamics simulation of a mixture of the Gay–Berne fluid and the Lennard-Jones fluid

Sten Sarman* and Aatto Laaksonen

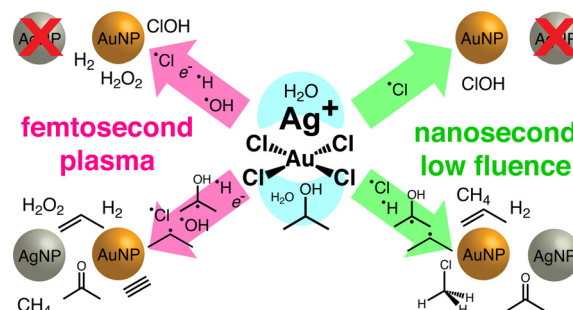


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Understanding photochemical pathways of laser-induced metal ion reduction through byproduct analysis

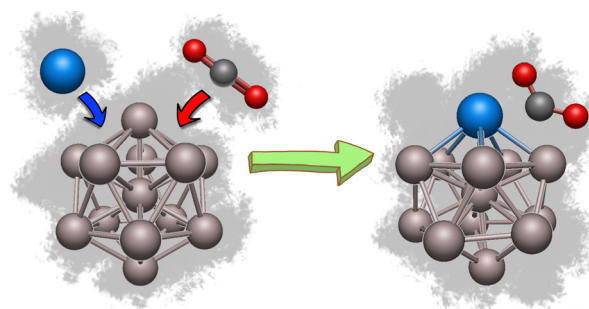
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Wave function analyses of scandium-doped aluminium clusters, Al_nSc ($n = 1-24$), and their CO₂ fixation abilities

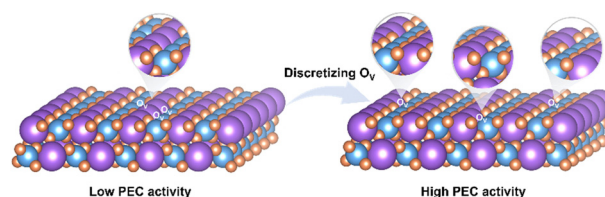
José Manuel Guevara-Vela, Arturo Sauza-de la Vega, Miguel Gallegos, Ángel Martín Pendás and Tomas Rocha-Rinza*



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Enhancing the photoelectrochemical activity of monoclinic BiVO₄ by discretizing oxygen vacancies: insights from DFT calculations

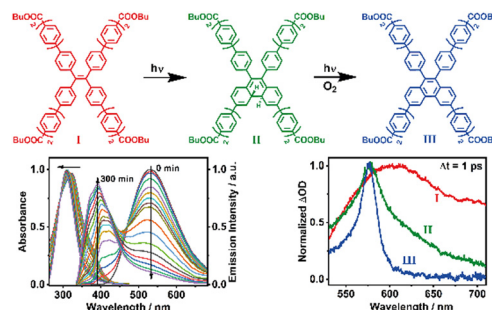
Shuyi Li, Xiaodan Yan and Jinlu He*



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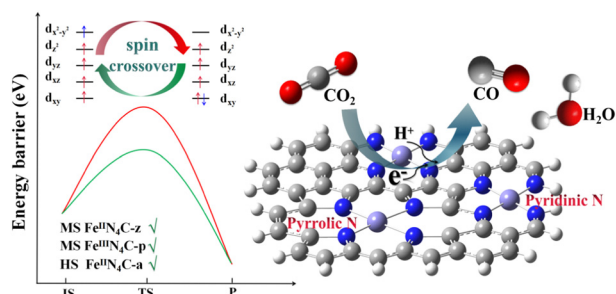
Photocyclization reaction and related photodynamics in the photoproducts of a tetraphenylethylene derivative with bulky substituents: unexpected solvent viscosity effect

Mario de la Hoz Tomás, Mao Yamaguchi, Boiko Cohen, Ichiro Hisaki and Abderrazzak Douhal*



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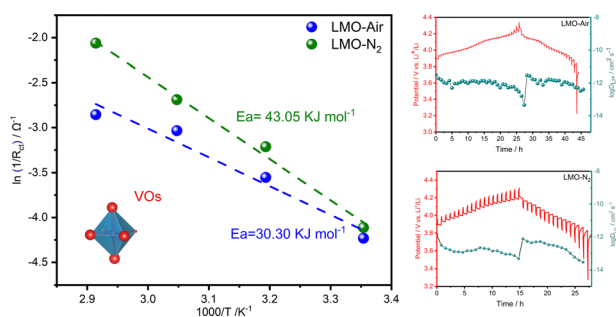
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The relationship between the local environment, N-type, spin state and catalytic functionality of carbon-hosted $\text{Fe}^{\text{II/III}}\text{-N}_4$ for the conversion of CO_2 to CO

Yuxin Xie, Yuning Yang, Wanping Yang, Nian Liu and Xiaohua Chen*

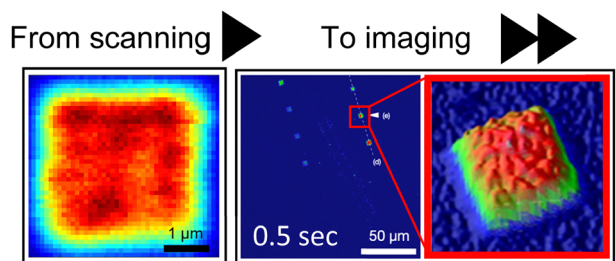
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The role of oxygen vacancies in the performance of LiMn_2O_4 spinel cathodes for lithium-ion batteries

Jing Wang, Haiyang Xing, Wenqiang Hou and Youlong Xu*

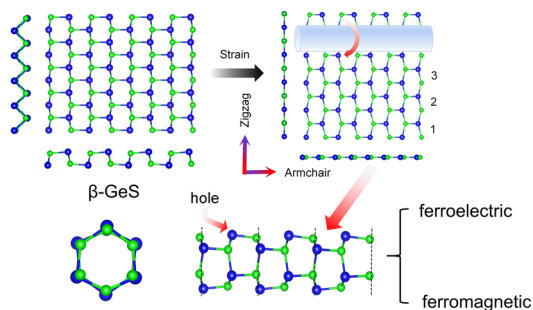
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Second harmonic generation from aluminum plasmonic nanocavities: from scanning to imaging

Tchiya Zar, Alon Krause, Omer Shavit, Hannah Aharon, Racheli Ron, Martin Oheim and Adi Salomon*

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Coexistence of ferroelectricity and ferromagnetism in hex-GeS nanowires

Jiajun Zhu, Heyun Zhao* and Wanbiao Hu*

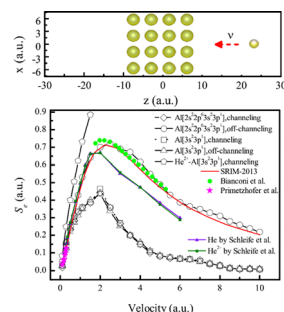


RESEARCH PAPERS

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Effects of semicore electrons on stopping power in helium-irradiated aluminum nanosheets

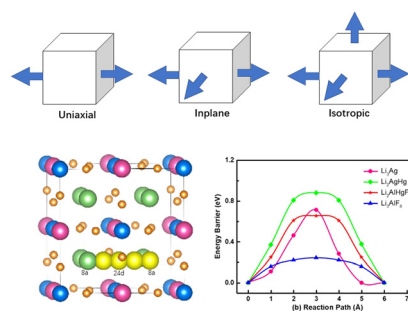
Su-Na Pang, Feng Wang,* Ya-Ting Sun, Fei Mao* and Cong-Zhang Gao*



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Strain effects on lithium ion diffusion in various crystal structures

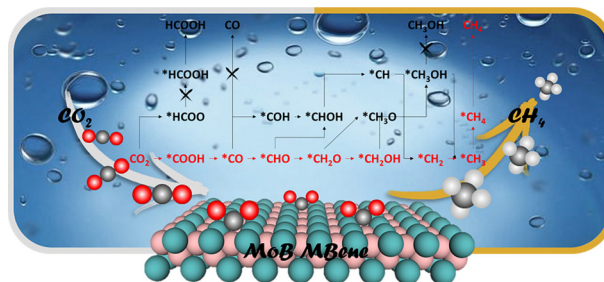
Bicong Liu, Jiamin Guo and Xiao Gu*



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Two-dimensional MBene: a comparable catalyst to MXene for effective CO_2 RR towards C_1 products

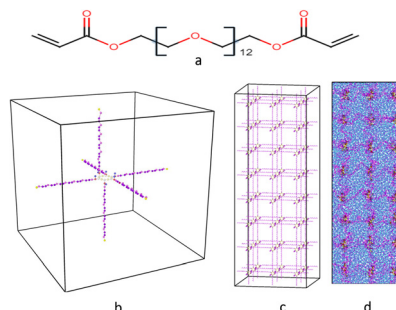
Xiaoqing Lu,* Yuying Hu, Shoufu Cao, Jiao Li, Chunyu Yang, Zengxuan Chen, Shuxian Wei,* Siyuan Liu and Zhaojie Wang*



18960

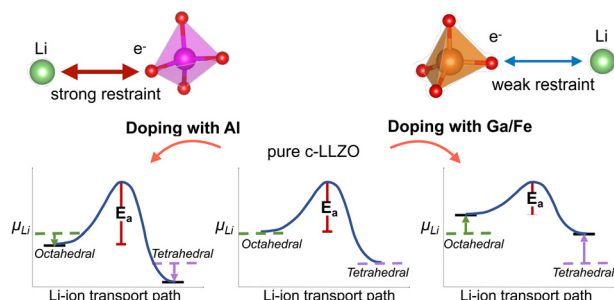
Effect of the degree of polymerization and water content on the thermal transport phenomena in PEGDA hydrogel: a molecular-dynamics-based study

Raju Kumar and Avinash Parashar*



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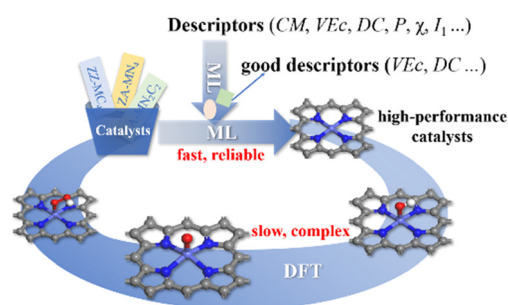
18973



Dopant-induced modulation of lithium-ion conductivity in cubic garnet solid electrolytes: a first-principles study

Feye-Feng Lu and Hong-Kang Tian*

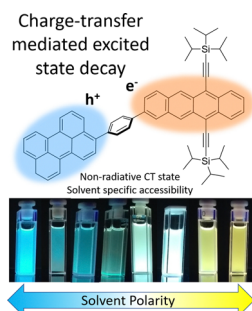
18983



The rational design of high-performance graphene-based single-atom electrocatalysts for the ORR using machine learning

Ziqiang Chen, Hexiang Qi, Haohao Wang, Caiwei Yue, Yangqiu Liu, Zuoyin Yang,* Min Pu and Ming Lei*

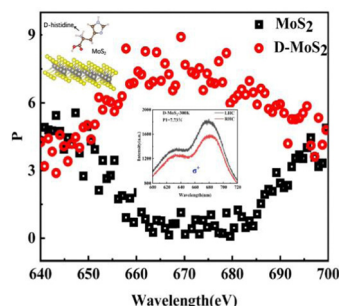
18990



Tuneable emission in single molecule dyads mediated by a charge transfer state

Matthew W. Brett, Michael B. Price, Calum K. Gordon, Karen E. Thorn, Lara D. Browne, Paul A. Hume, Justin M. Hodgkiss, Bridget L. Stocker, Mattie S. M. Timmer and Nathaniel J. L. K. Davis*

18998



Chiral molecule induced valley polarization enhancement of MoS₂

Guangcun Gao, Jintong Zhu, Songrui Wei, Yang Cao, Wei Huang, Zhongxin Liu, Jieqiong Wang* and Yijun Shen*

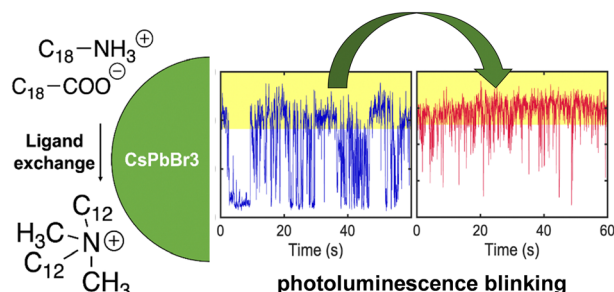


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19004

Suppression of blinking in single CsPbBr₃ perovskite nanocrystals through surface ligand exchange

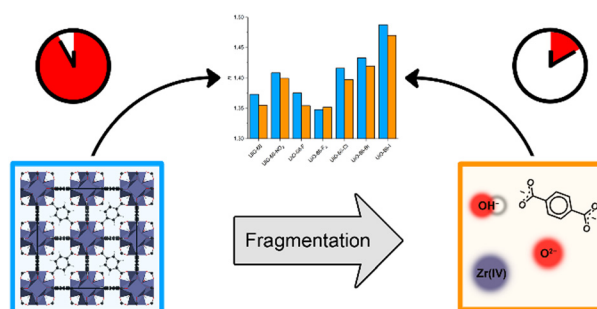
Toranosuke Takagi, Shun Omagari and Martin Vacha*



19013

Fragment-based approach for the efficient calculation of the refractive index of metal–organic frameworks

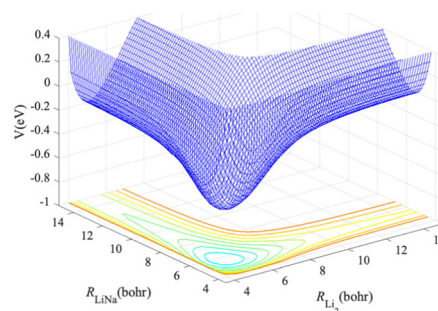
Marvin Treger, Carolin König, Peter Behrens and Andreas M. Schneider*



19024

A neural network potential energy surface for the Li + LiNa → Li₂ + Na reaction and quantum dynamics study from ultracold to thermal energies

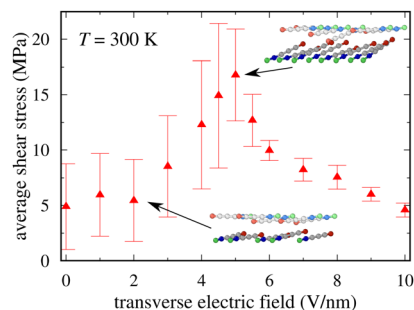
Bayaer Buren



19037

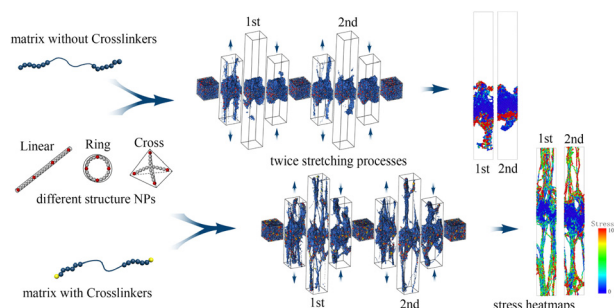
Electric-field frictional effects in confined zwitterionic molecules

Melisa M. Gianetti, Roberto Guerra, Andrea Vanossi, Michael Urbakh and Nicola Manini*



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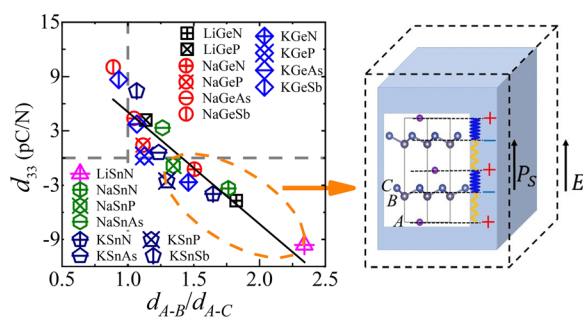
19046



Molecular dynamics simulation insight into topological structure dependence of self-healing polymer nanocomposites

Wei Shang, Guanyi Hou,* Runhan Ren, Xinyu Li, Yunxuan Weng* and Jun Liu

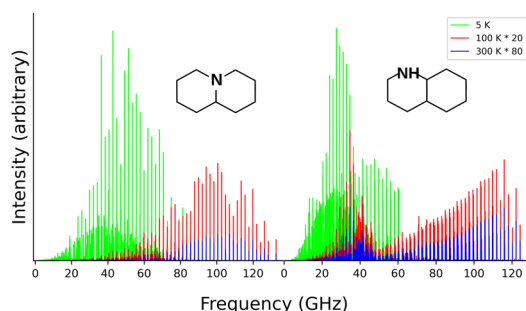
19058



Origin of the negative longitudinal piezoelectric effect and electric auxetic effect in hexagonal $A^I B^IV C^V$ semiconductors

Ling-Xu Zhao and Jian Liu*

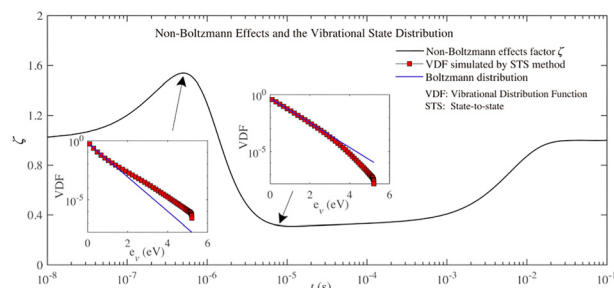
19066



Theoretical microwave spectra of interstellar nitrogen-containing PAHs

Akant Vats, Satyam Srivastav, Anshika Pandey and Amit Pathak*

19073



Vibrational non-Boltzmann effects on the dissociation rate of oxygen

Rui Xiong, Yufeng Han and Wei Cao*

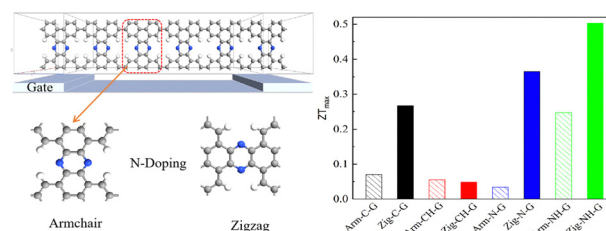


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19082

Anisotropic thermoelectric properties in hydrogenated nitrogen-doped porous graphene nanosheets

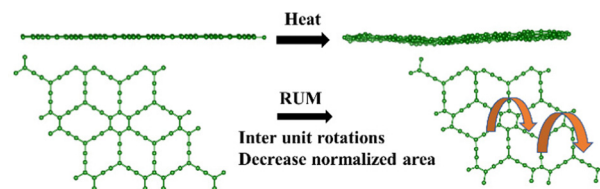
Xia Yu, Jun-hua Liu,* Wu-Xing Zhou, Zhong-Xiang Xie, Pin-Zhen Jia, Yuan-Xiang Deng, Xuan-Hao Cao, Zhi-Qiang Fan and Dan Wu*



19091

Biaxial negative thermal expansion in carbon nets – graphyne and derivatives

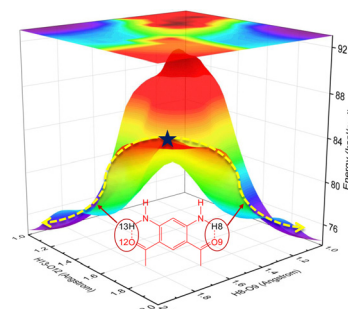
Soumya Mondal and Ayan Datta*



19098

Non-adiabatic dynamics simulations of the S_1 excited-state relaxation of diacetyl phenylenediamine

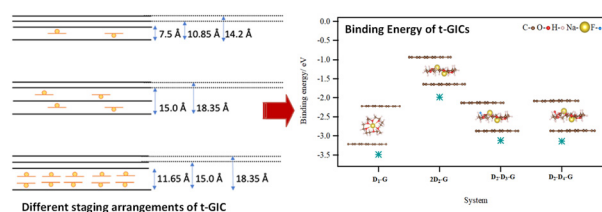
Xiaohang Chen, Wei Wang, Dongyi Xiao, Shu-Hua Xia* and Yan Zhang*



19106

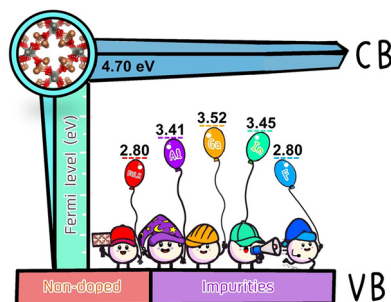
Effect of fluoro and hydroxy analogies of diglyme on sodium-ion storage in graphite: a computational study

R. M. N. M. Rathnayake, Debra J. Searles, Timothy T. Duignan and X. S. Zhao*



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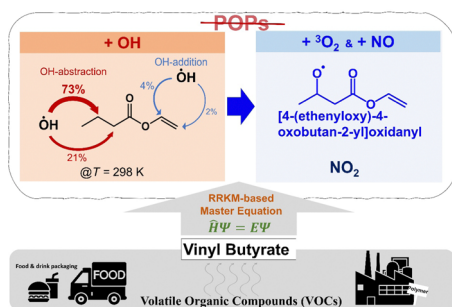
19116



The role of native point defects and donor impurities in the electrical properties of ZnSb_2O_4 : a hybrid density-functional study

Supparat Charoenphon, Auttasit Tubtimtae, Isao Watanabe, Sirichok Jungthawan, Jiraroj T-Thienprasert, Adisak Boonchun and Pakpoom Reunchan*

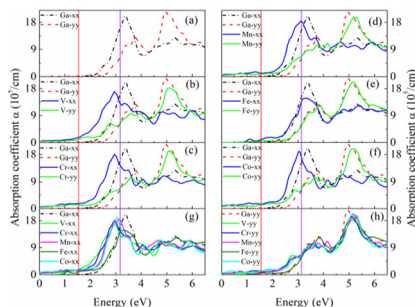
19126



OH-initiated oxidation of vinyl butyrate: *ab initio* insights

Loc T. Nguyen, Uyen N.-P. Tran, Tam V.-T. Mai, Trang T. Nguyen and Lam K. Huynh*

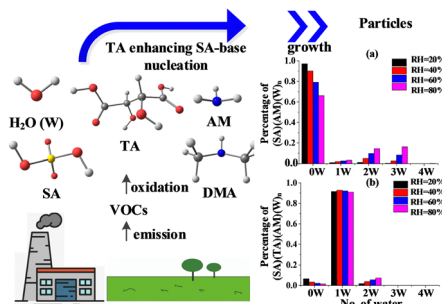
19139



Theoretical investigation of the magnetic and optical properties in a transition metal-doped GaTeCl monolayer

Pengxia Zhou,* Ziheng Pan, Qian Gao, Qian Zou, Jieru Sun, Yinxin Li, You Qian, Shang Li, Chonggui Zhong,* Lihua Qu and Zhengchao Dong

19147



Enhancing acid–base–water ternary aerosol nucleation with organic acid: a case of tartaric acid

Chunyu Wang, Jiayun Zhao, Xiaoju Chen, Renyi Zhang* and Shuai Jiang*

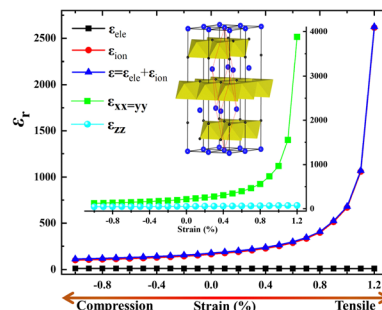


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19158

Strain-induced giant enhancement of anisotropic dielectric constant in layered nitrides SrHfN_2 and SrZrN_2

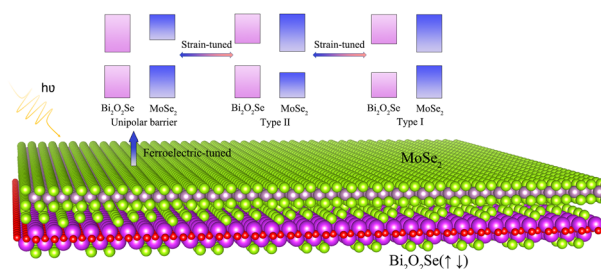
Min Yao, Yuanyun Zhang, Jianmin Ban, Junjie Hou, Bowen Zhang, Junwei Liu, Xing Ming* and Xiaojun Kuang*



19167

Ferroelectric and strain-tuned $\text{MoSe}_2/\text{Bi}_2\text{O}_2\text{Se}$ van der Waals heterostructure with band alignment evolution

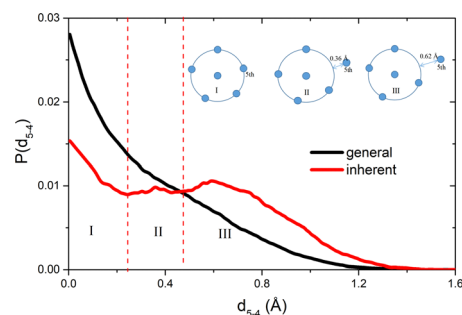
Shucao Lu, Yanlu Li* and Xian Zhao*



19175

Inherent structures of water using fully *ab initio* simulations

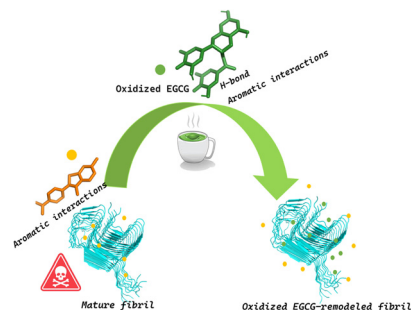
Shuo Cao, Gang Zhao* and Dehua Wang



19182

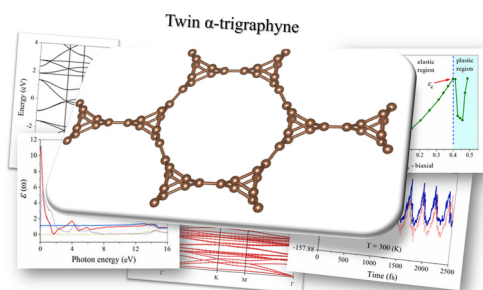
How oxidized EGCG remodels α -synuclein fibrils into non-toxic aggregates: insights from computational simulations

Priscila Baltazar Gonçalves*, Fernando L. Palhano, Yraima Cordeiro and Ana Carolina Rennó Soderó*



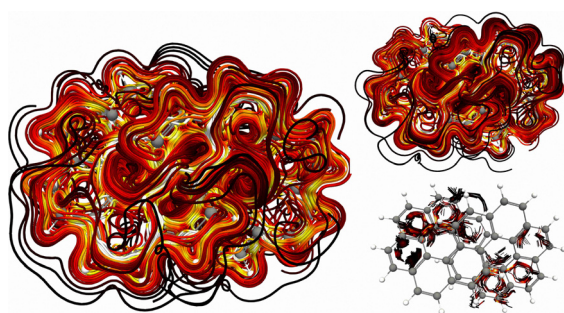
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19195

**Twin α -trigraphyne: a new two-dimensional carbon material**

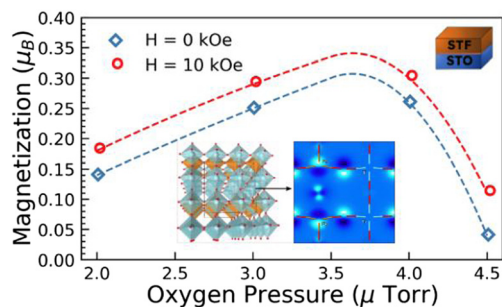
Roya Majidi* and Marzieh Nadafan

19207

**The magnetically induced current density of the [12]infinittene dianion**

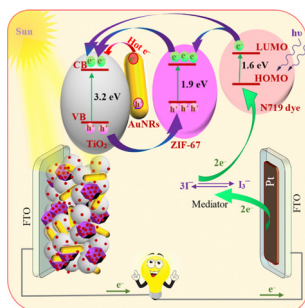
Qian Wang, Mesías Orozco-Ic and Dage Sundholm*

19214

**First-principles based Monte Carlo modeling of the magnetization of oxygen-deficient Fe-substituted SrTiO_3**

Juan M. Florez,* Miguel A. Solís, Emilio A. Cortés Estay, E. Suárez Morell and Caroline A. Ross

19230

**AuNRs attached TiO_2 NPs modified by cobalt-imidazolate frameworks as exceptional materials to improve the energy conversion efficiency of dye-sensitized solar cells**

Nafiseh Bagheri, Javad Hassanzadeh, Zainab B. Al-Rugeishi, Ninie Suhana Abdul Manan, Haider A. J. Al Lawati and Osama K. Abou-Zied*

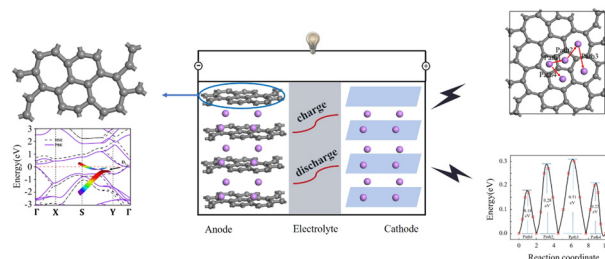


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19239

LC₅₆₇: a new 2D semimetallic carbon allotrope as a promising anode material for lithium-ion batteries

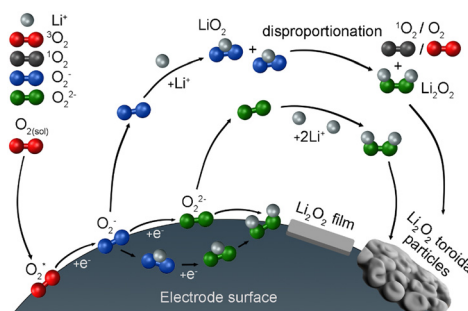
Yusheng Cai, Yi Wei, Cuihong Lv,* Lichuan Zhang* and Yuanping Chen



19245

Mixture of an ionic liquid and organic solvent at graphene: interface structure and ORR mechanism

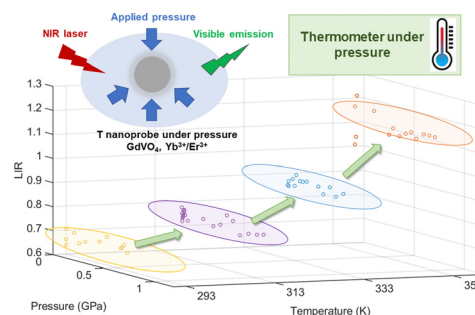
Sergey Pavlov* and Sergey Kislenco



19254

Er³⁺ doped nanoparticles as upconversion thermometer probes in confined fluids

Yujiao Zhou, Gilles Ledoux, Laurence Bois,* Sylvie Descartes, Nathalie Bouscharain, Fernand Chassagneux, Matteo Martini, Yamaldi Midiladji Bakary, Catherine Journet and David Philippon*



CORRECTIONS

19266

Correction: Automated assessment of redox potentials for dyes in dye-sensitized photoelectrochemical cells

Jelena Belić, Arno Förster, Jan Paul Menzel, Francesco Buda and Lucas Visscher*



CORRECTIONS

19269

Correction: Terahertz spectroscopy of the helium endofullerene He@C₆₀

Tanzeeha Jafari, George Razvan Bacanu, Anna Shugai, Urmas Nagel, Mark Walkey, Gabriela Hoffman, Malcolm H. Levitt, Richard J. Whitby and Toomas Rõõm*

19270

Correction: The Li + CaF → Ca + LiF chemical reaction under cold conditions

Humberto da Silva Jr, Qian Yao, Masato Morita, Brian K. Kendrick, Hua Guo* and Naduvalath Balakrishnan*

19271

Correction: Tuning the melting point of selected ionic liquids through adjustment of the cation's dipole moment

Brooks D. Rabideau,* Mohammad Soltani, Rome A. Parker, Benjamin Siu, E. Alan Salter, Andrzej Wierzbicki, Kevin N. West and James H. Davis Jr*

