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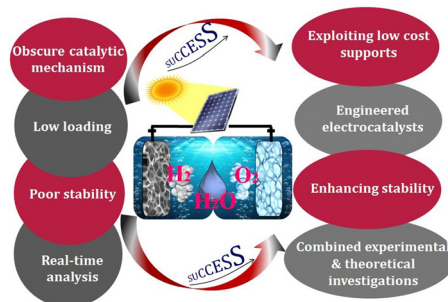
See Fei Mao *et al.*,
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Phys. Chem. Chem. Phys.,
2023, 25, 9043.

REVIEW

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Research on engineered electrocatalysts for efficient water splitting: a comprehensive review

Jayaraman Jayabharathi,* Balakrishnan Karthikeyan, Bakthavachalam Vishnu and Sundarraj Sriram

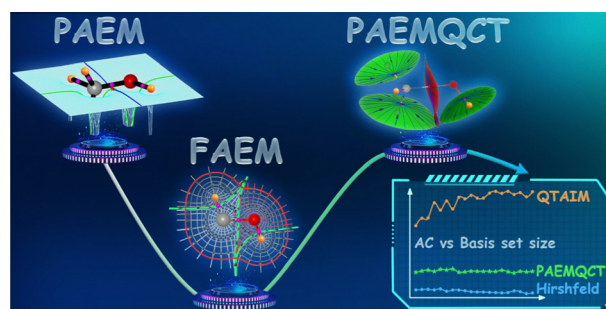


PERSPECTIVE

9020

Atomic charges in molecules defined by molecular real space partition into atomic subspaces

Jian Zhao, Zun-Wei Zhu, Dong-Xia Zhao* and Zhong-Zhi Yang*



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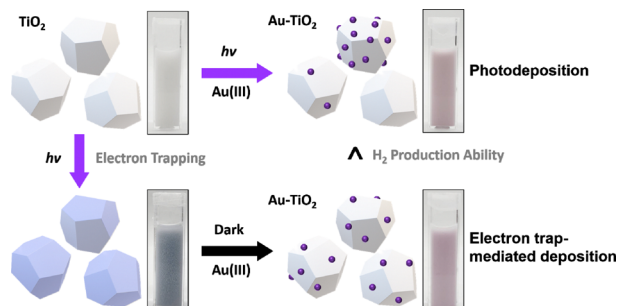


COMMUNICATIONS

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Well-dispersed Au co-catalyst deposited on a rutile TiO₂ photocatalyst *via* electron traps

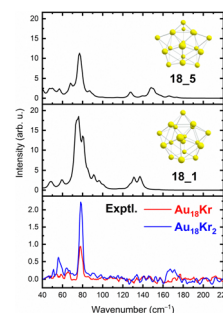
Tomoki Akiyama, Haruki Nagakawa and Tetsu Tatsuma*



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A new look at the structure of the neutral Au₁₈ cluster: hollow versus filled golden cage

Pham Vu Nhat,* Nguyen Thanh Si, André Fielicke, Vitaly G. Kiselev and Minh Tho Nguyen*

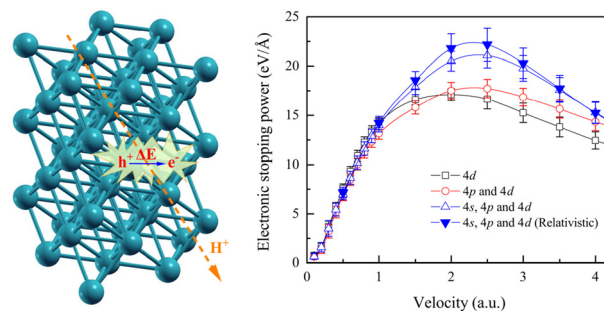


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The contribution of inner electron excitation to the electronic stopping power of palladium for protons

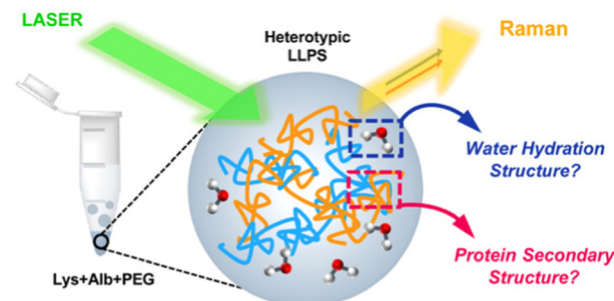
Wen-Qi Jin, Fei Mao,* Shi-Ming Li, Wen-Qi Zuo, Rui-Da Chen, Ge-Ge Xiong, Hong Mao, Feng Wang and Feng-Shou Zhang



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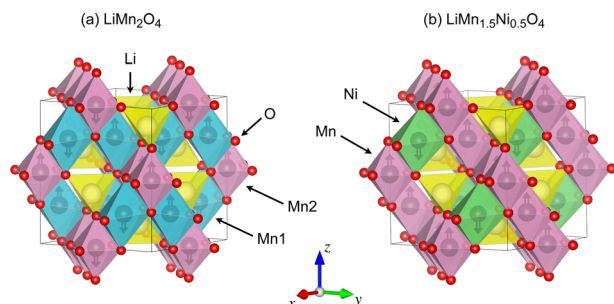
Micro-Raman spectroscopic analysis of liquid–liquid phase separation

Suin Choi, So Yeon Chun, Kyungwon Kwak* and Minhaeng Cho*



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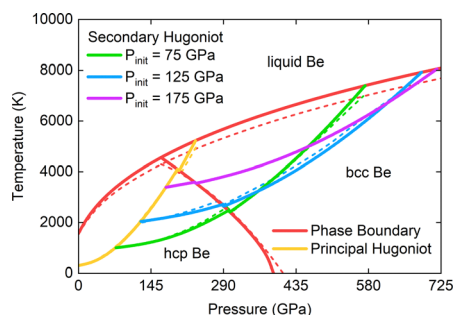
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Unraveling the effects of inter-site Hubbard interactions in spinel Li-ion cathode materials

Iurii Timrov,* Michele Kotiuga and Nicola Marzari

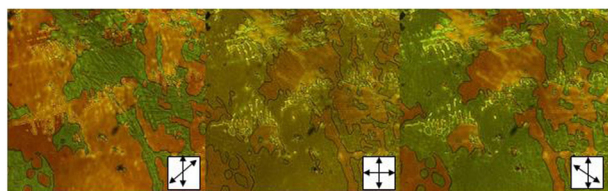
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Toward better understanding of the high-pressure structural transformation in beryllium by the statistical moment method

Tran Dinh Cuong* and Anh D. Phan

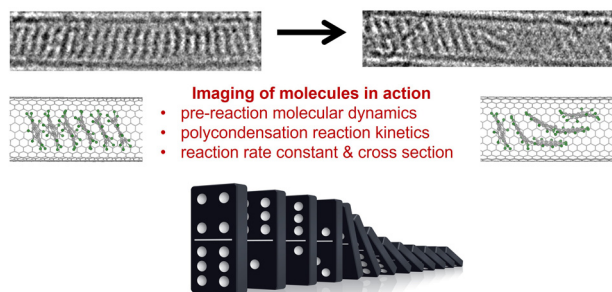
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Spontaneous mirror symmetry breaking and chiral segregation in the achiral ferronematic compound DIO

Neelam Yadav, Yuri P. Panarin, Wanhe Jiang, Georg H. Mehl and Jagdish K. Vij*

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Direct measurement of single-molecule dynamics and reaction kinetics in confinement using time-resolved transmission electron microscopy

Kayleigh L. Y. Fung, Stephen T. Skowron, Ruth Hayter, Stephen E. Mason, Benjamin L. Weare, Nicholas A. Besley, Quentin M. Ramasse, Christopher S. Allen and Andrei N. Khlobystov*

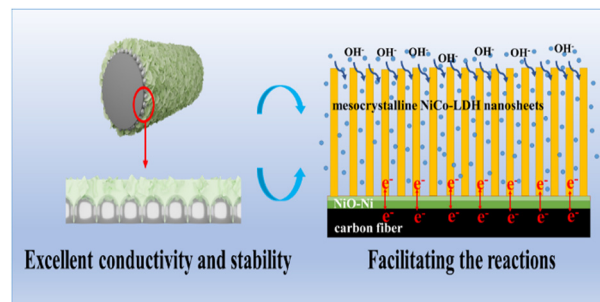


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Flexible aqueous supercapacitors with excellent cycling performance and high-energy density based on mesocrystalline NiCo-LDHs

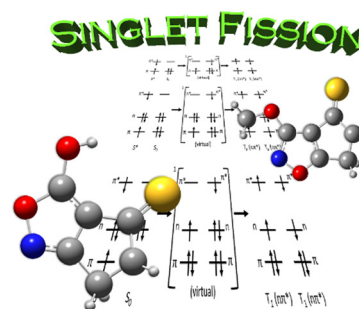
Xiaohui Xie, Jinyue Song, Hongguang Fan, Lichong Bai, Shuang Liu, Yanpeng Wang, Wansu Zheng and Wei Liu*



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Quest for singlet fission of organic sulfur-containing systems in the higher lying singlet excited state: application prospects of anti-Kasha's rule

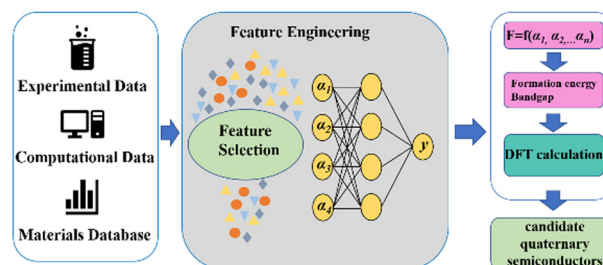
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Machine learning and density functional theory simulation of the electronic structural properties for novel quaternary semiconductors

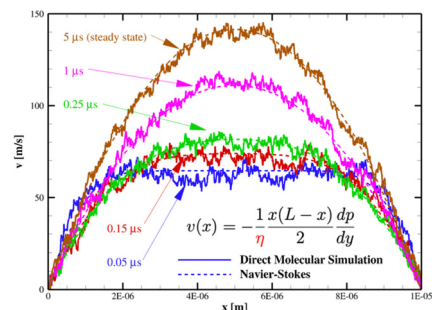
Mengwei Gao, Bo Cai,* Gaoyu Liu, Lili Xu, Shengli Zhang* and Haibo Zeng*



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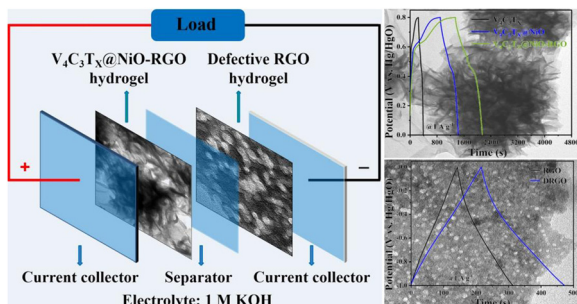
First-principles predictions for shear viscosity of air components at high temperature

Paolo Valentini,* Ashley M. Verhoff, Maninder S. Grover and Nicholas J. Bisek



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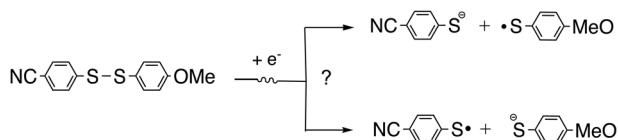
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Hierarchical $V_4C_3T_x@NiO$ -reduced graphene oxide heterostructure hydrogels and defective reduced graphene oxide hydrogels as free-standing anodes and cathodes for high-performance asymmetric supercapacitors

Ziyu Geng, Weiwen Chen, Zenghui Qiu,* Haijun Xu,* Dingjie Pan and Shaowei Chen*

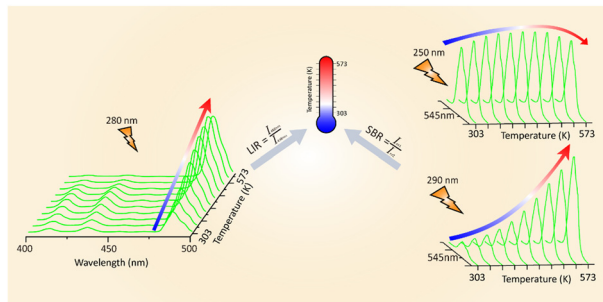
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Mesolysis of an asymmetric diphenyldisulfide radical anion studied by γ -ray and pulsed-electron radiolyses

Minoru Yamaji,* Sachiko Tojo, Tetsuro Majima and Mamoru Fujitsuka*

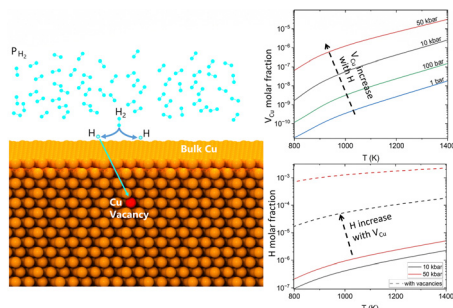
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Tb^{3+} -based multi-mode optical ratiometric thermometry

Zixuan Zhang, Fei Li,* Yuanbo Yang, Zhijun Wang, Panlai Li, Rongxiang Zhang,* Hao Suo and Leipeng Li*

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Thermodynamic analysis of the interaction between metal vacancies and hydrogen in bulk Cu

Vasileios Fotopoulos,* Ricardo Grau-Crespo and Alexander L. Shluger

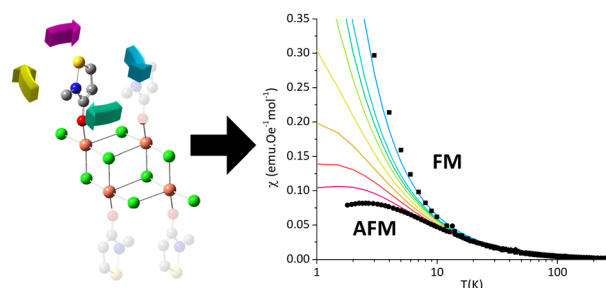


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Satellite ligand effects on magnetic exchange in dimers. A structural, magnetic and theoretical investigation of $\text{Cu}_2\text{L}_2\text{X}_4$ (L = methylisothiazolinone and $\text{X} = \text{Cl}^-$, Br^-)

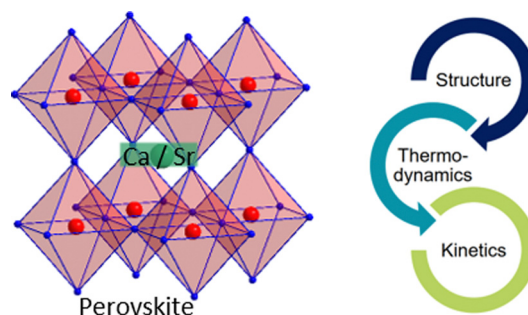
Stefan Coetzee, Mark M. Turnbull, Christopher P. Landee, Jeffrey C. Monroe, Mercè Deumal, Juan. J. Novoa and Melanie Rademeyer*



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Impact of the Sr content on the redox thermodynamics and kinetics of $\text{Ca}_{1-x}\text{Sr}_x\text{MnO}_{3-\delta}$ for tailored properties

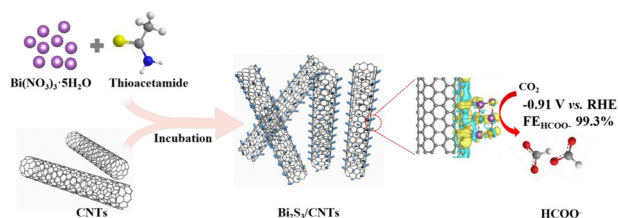
Lena Klaas,* Brendan Bulfin, Dorottya Kriechbaumer, Martin Roeb and Christian Sattler



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Bi_2S_3 nanorods grown on multiwalled carbon nanotubes as highly active catalysts for CO_2 electroreduction to formate

Fangfang Yang, Zailai Xie, Xuke Huang, Xiangyang Yin, Weifeng Zhang, Yongkui Huang and Daijun Zhang*

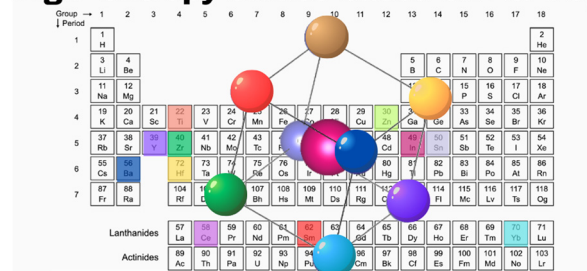


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Water uptake and energetics of the formation of barium zirconate based multicomponent oxides

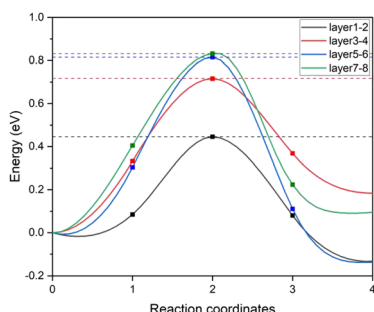
Aleksandra Mielewczyk-Gryn,* Tamilarasan Subramani,* Daniel Jaworski, Kristina Lilova, Wojciech Skubida, Alexandra Navrotsky and Maria Gazda

High entropy oxides based on BaZrO_3



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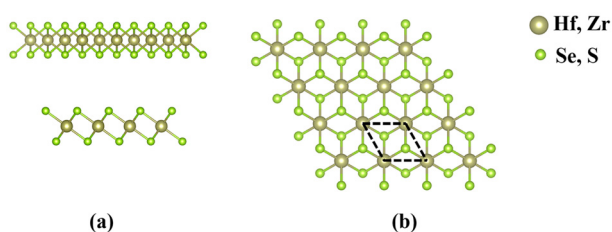
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Oxygen migration performance of LaFeO₃ perovskite-type oxygen carriers with Sr doping

Yuan Feng, Hanyu Jin and Shuai Wang*

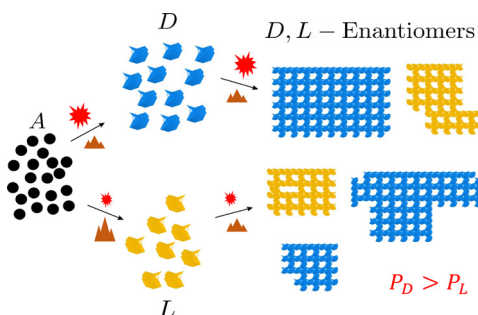
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Tensile strain and finite size modulation of low lattice thermal conductivity in monolayer TMDCs (HfSe₂ and ZrS₂) from first-principles: a comparative study

Guofu Chen, Wenlong Bao, Zhaoliang Wang* and Dawei Tang

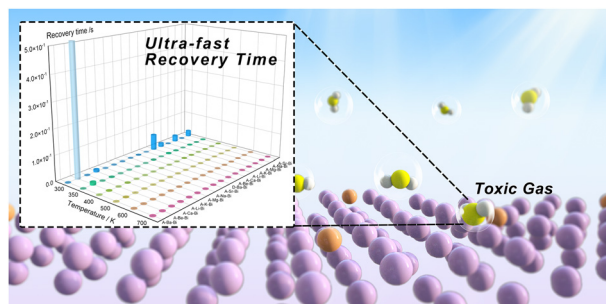
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Chiral symmetry breaking induced by energy dissipation

A. Arango-Restrepo,* O. Arteaga, D. Barragán and J. M. Rubi

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Single atom modified two-dimensional bismuthenes for toxic gas detection

An Chen, Yanqiang Han, Zhilong Wang, Junfei Cai, Simin Ye and Jinjin Li*

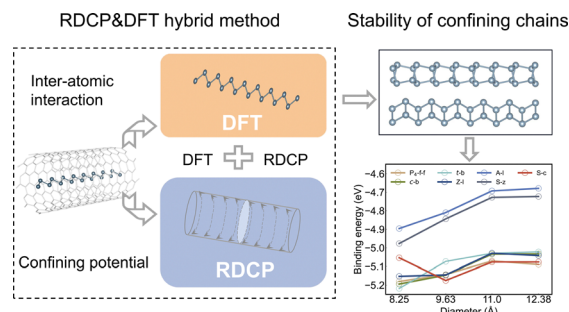


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Towards an accurate description of one-dimensional pnictogen allotropes in nano-confinements

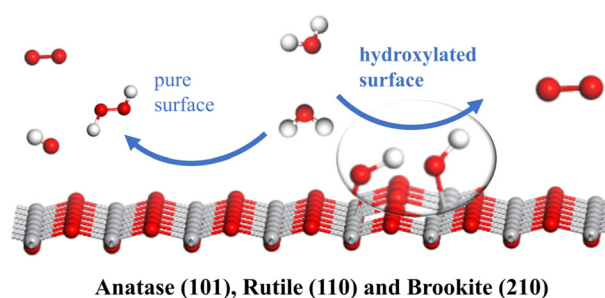
Jing Chang,* Tonghuan Jiang, Wei Fang and Ji Chen



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Tuning the water-splitting mechanism on titanium dioxide surfaces through hydroxylation

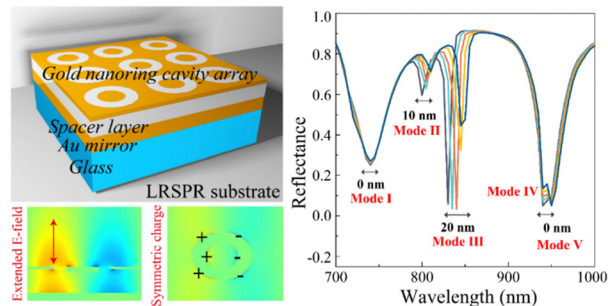
Lu Wu, Meijing Liao, Bing Zhao, Qianni Li, Bin Liu* and Yuexing Zhang*



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High-sensitivity long-range surface plasmon resonance sensing assisted by gold nanoring cavity arrays and nanocavity coupling

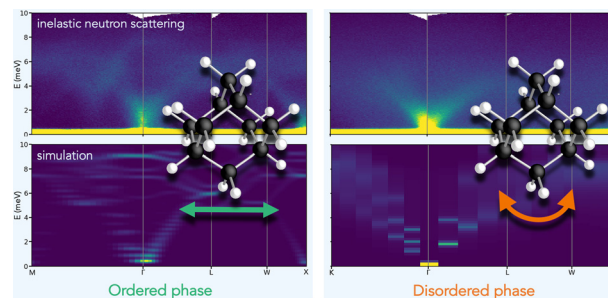
Xiaojun Luo, Rui Tan, Qiuju Li, Jiaxin Chen, Yalin Xie, Jiayi Peng, Mei Zeng, Minghang Jiang,* Caijun Wu* and Yi He*



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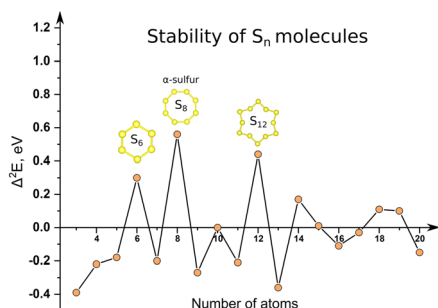
Dynamics in the ordered and disordered phases of barocaloric adamantane

Bernet E. Meijer, Richard J. C. Dixey, Franz Demmel, Robin Perry, Helen C. Walker* and Anthony E. Phillips*



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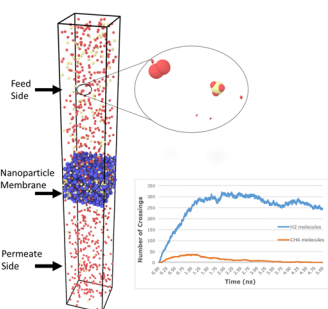
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Stability of sulfur molecules and insights into sulfur allotropy

Maria Fedyaeva,* Sergey Lepeshkin and Artem R. Oganov

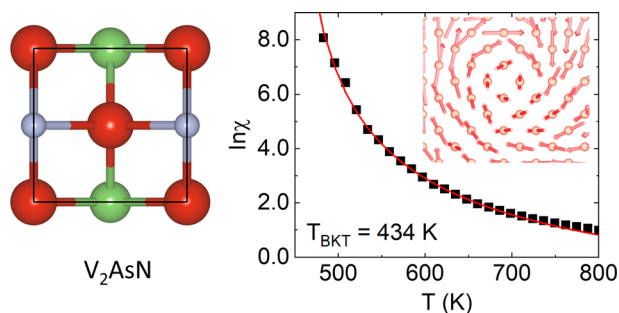
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Realizing high performance gas filters through nano-particle deposition

Dhruva Patil and Tribikram Gupta*

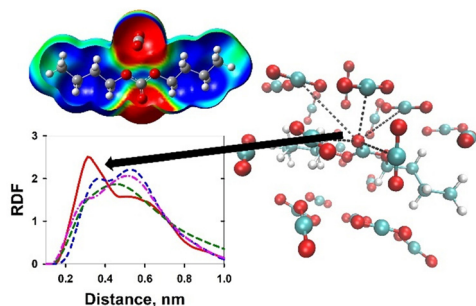
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Two-dimensional XY ferromagnetism above room temperature in Janus monolayer V₂XN (X = P, As)

Wenhui Wan, Botao Fu, Chang Liu, Yanfeng Ge and Yong Liu*

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Chemical similarity of dialkyl carbonates and carbon dioxide opens an avenue for novel greenhouse gas scavengers: cheap recycling and low volatility *via* experiments and simulations

Vitaly V. Chaban,* Nadezhda A. Andreeva, Franciele L. Bernard, Leonardo M. dos Santos and Sandra Einloft

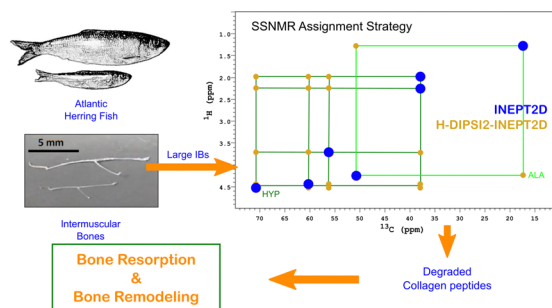


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Investigating bone resorption in Atlantic herring fish intermuscular bones with solid-state NMR

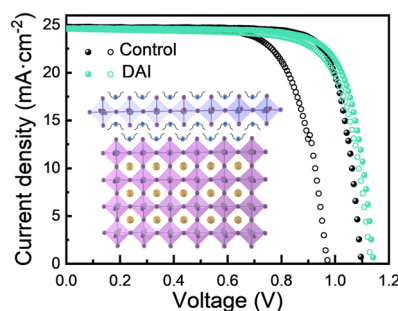
Hsin Wang,* Steve Falcoz, Jorge Morales and Jean-Philippe Berteau



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In situ surface regulation of 3D perovskite using diethylammonium iodide for highly efficient perovskite solar cells

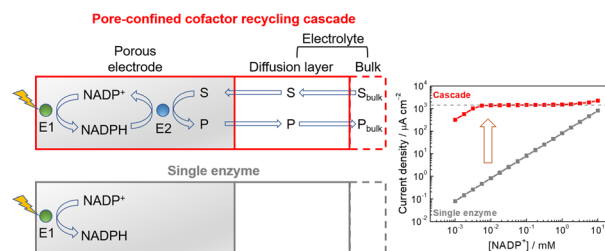
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Design principles for a nanoconfined enzyme cascade electrode via reaction–diffusion modelling

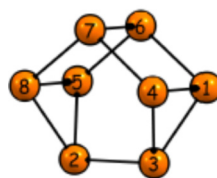
Bhavin Siritanaratkul



9364

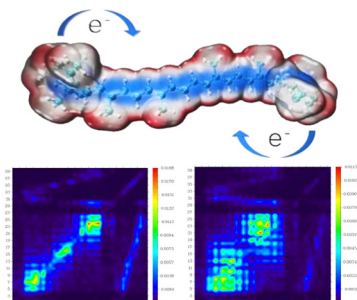
Aromaticity in P₈ allotropes and (CH)₈ analogues: significance of their 40 valence electrons?

Amr A.A. Attia, Alvaro Muñoz-Castro, Alexandru Lupan* and R. Bruce King*

P₈ cuneane(CH)₈
cyclooctatetraene

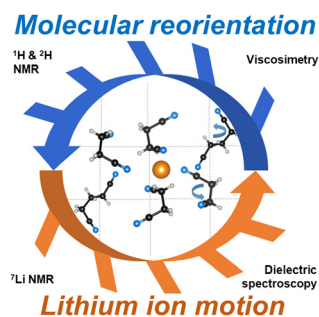
RESEARCH PAPERS

9373

Exploring electronic energy level structure and excited electronic states of β -carotene using DFT

Lu Xing, Zhenguo Dou, Xiumian Cao, Panpan Ren, Wei Zhang, Shenghan Wang,* Chenglin Sun* and Zhiwei Men*

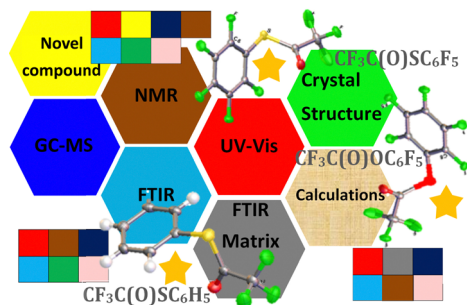
9382



Paddle-wheel mechanism in doped succinonitrile–glutaronitrile plastic electrolyte: a joint magnetic resonance, dielectric, and viscosimetry study of Li ion translational and molecular reorientational dynamics

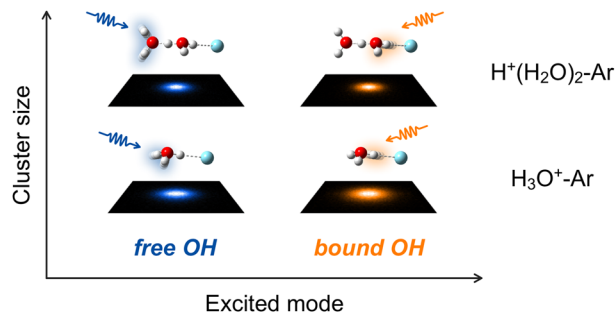
S. Lansab,* B. Grabe and R. Böhmer

9394

Spectroscopic and structural studies on phenyl and pentafluorophenyl trifluorothioacetate, and pentafluorophenyl trifluoroacetate, $\text{CF}_3\text{C}(\text{O})\text{SC}_6\text{H}_5$, $\text{CF}_3\text{C}(\text{O})\text{SC}_6\text{F}_5$ and $\text{CF}_3\text{C}(\text{O})\text{OC}_6\text{F}_5$

Vanina M. Cayón, Mauricio F. Erben,* Rosana M. Romano, Hans-Georg Stammer, Norbert W. Mitzel* and Carlos O. Della Védova*

9404

Fragment imaging in the infrared photodissociation of the Ar-tagged protonated water clusters $\text{H}_3\text{O}^+-\text{Ar}$ and $\text{H}^+(\text{H}_2\text{O})_2-\text{Ar}$

Yuri Ito, Mizuhiro Kominato, Yuji Nakashima, Keijiro Ohshimo and Fuminori Misaizu*

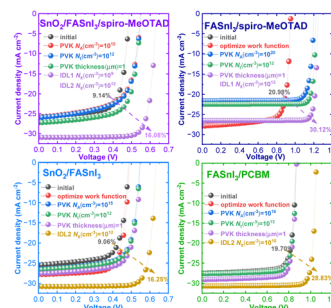


RESEARCH PAPERS

9413

Rational design of formamidine tin-based perovskite solar cell with 30% potential efficiency via 1-D device simulation

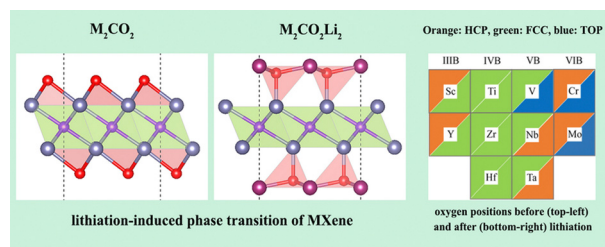
Kaiwen Liang, Like Huang,* Tianzhou Wang, Chaofeng Wang, Yi Guo, Yunliang Yue, Xiaohui Liu, Jing Zhang, Ziyang Hu and Yuejin Zhu*



9428

A systematic computational investigation of lithiation-induced structural phase transitions of O-functionalized MXenes

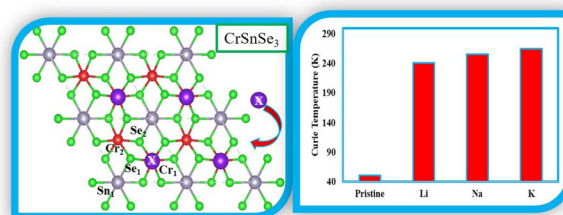
Qianku Hu,* Yuhuan Ji, Dandan Li, Zhe Wang, Kun Han, Qinghua Wu, Junkai Wang, Qixun Xia, Libo Wang and Aiguo Zhou*



9437

Enhanced Curie temperature in partially decorated CrSnSe₃ monolayer with alkali metals (Li, Na, and K)

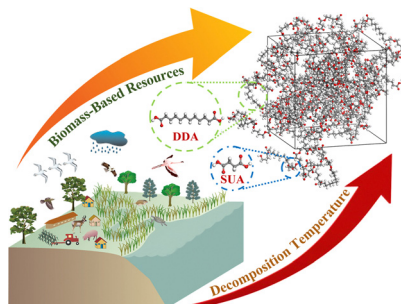
Imran Khan and Jisang Hong*



9445

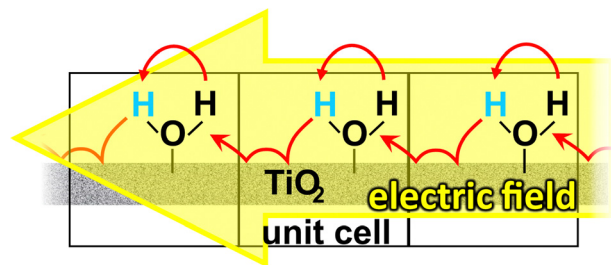
ReaxFF molecular dynamics simulation of the thermal decomposition reaction of bio-based polyester materials

Xinyu Li, Yue Han, Jiajun Qu, Qionghai Chen, Yuan Wei, Guanyi Hou* and Jun Liu*



RESEARCH PAPERS

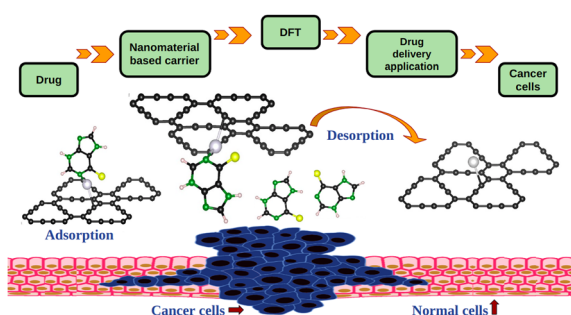
9454



First-principles study on unidirectional proton transfer on anatase TiO_2 (101) surface induced by external electric fields

Takahiro Chiba, Kenji Iida,* Shinya Furukawa and Jun-ya Hasegawa

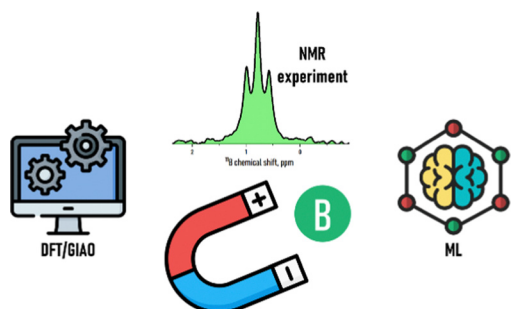
9461



Metal-decorated γ -graphyne as a drug transporting agent for the mercaptopurine chemotherapy drug: a DFT study

Sreejith Pallikkara Chandrasekharan, Seetha Lakshmy, Gopal Sanyal, Nandakumar Kalarikkal,* Ravi Trivedi and Brahmananda Chakraborty*

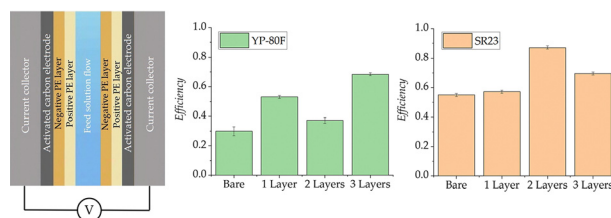
9472



Accurate prediction of ^{11}B NMR chemical shift of BODIPYs via machine learning

Alexander A. Ksenofontov,* Yaroslav I. Isaev, Michail M. Lukanov, Dmitry M. Makarov, Varvara A. Eventova, Ilya A. Khodov* and Mechail B. Berezin

9482



Effects of layer-by-layer coating on activated carbon electrodes for capacitive deionization

Sergio Orozco-Barrera, Guillermo R. Iglesias, Ángel V. Delgado, Sergio García-Larios and Silvia Ahualli*

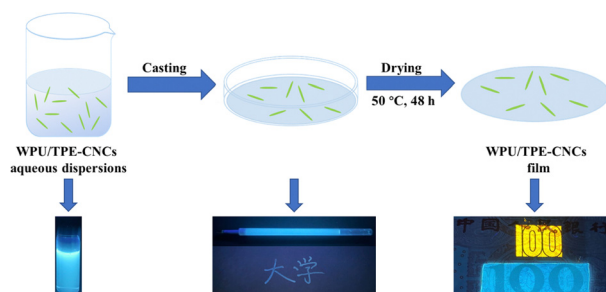


RESEARCH PAPERS

9492

Fluorescent cellulose nanocrystals/waterborne polyurethane nanocomposites for anti-counterfeiting applications

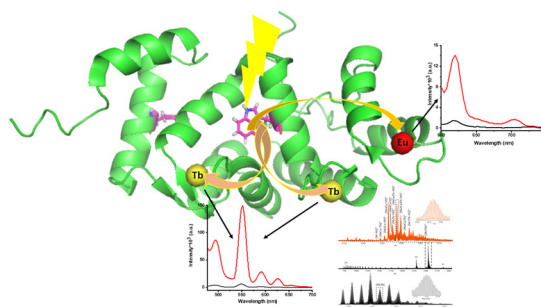
Xiu Ye, Sai Wang, Peng Zhou,* Dongyang Zhang* and Pengli Zhu*



9500

Distinct mechanism of Tb³⁺ and Eu³⁺ binding to NCS1

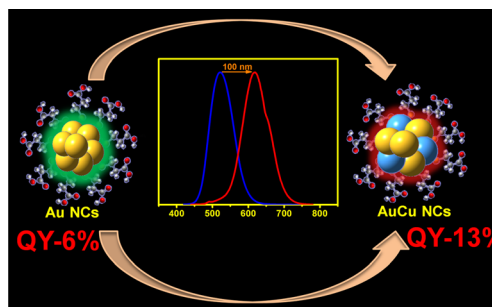
Md Shofiul Alam, Dennys Leyva, Woodline Michelin, Francisco Fernandez-Lima and Jaroslava Miksovska*



9513

Experimental and computational insights into luminescence in atomically precise bimetallic Au_{6-n}Cu_n(MPA)₅ (n = 0–2) clusters

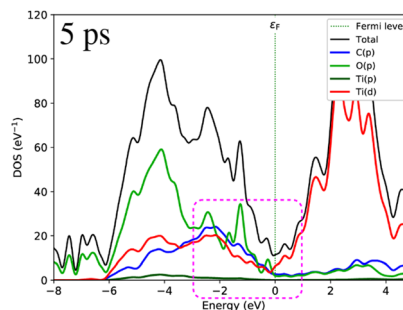
Aarti Devi, Harshita Seksaria, Dipankar Bain, Sarita Kolay, Rashi, Abir De Sarkar* and Amitava Patra*



9522

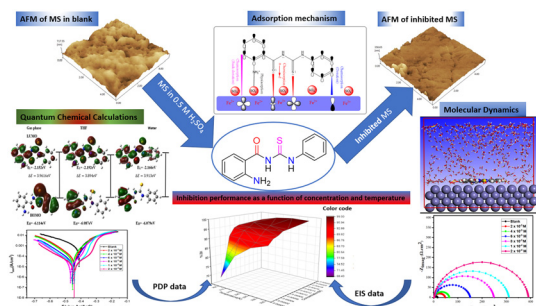
Photo-response of water intercalated Ti₃C₂O₂ MXene

Junais Habeeb Mekkath



RESEARCH PAPERS

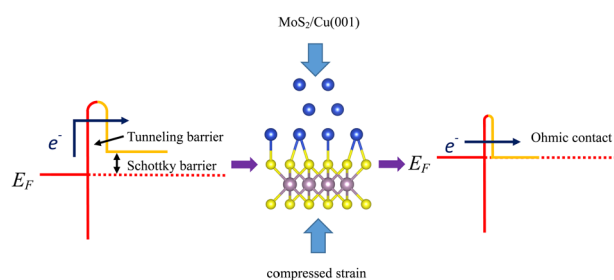
9532



Synthesis, DFT, molecular dynamics, and Monte Carlo simulation of a novel thiourea derivative with extraordinary inhibitive properties for mild steel in 0.5 M sulphuric acid

Ahmed M. Hegazy, Nesreen S. Haiba, Mohamed K. Awad* and Fatma M. Mahgoub

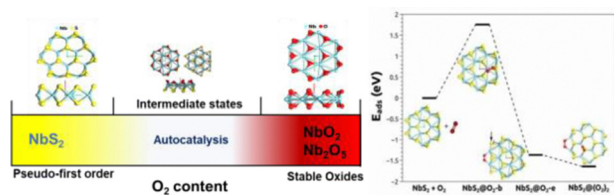
9548



Interfacial contact barrier and charge carrier transport of MoS₂/metal(001) heterostructures

Zi-Wen Zhang, Zhao-Sheng Liu, Jun-Jie Zhang, Bing-Ning Sun, Dai-Feng Zou, Guo-Zheng Nie, Mingyan Chen, Yu-Qing Zhao* and Shaolong Jiang*

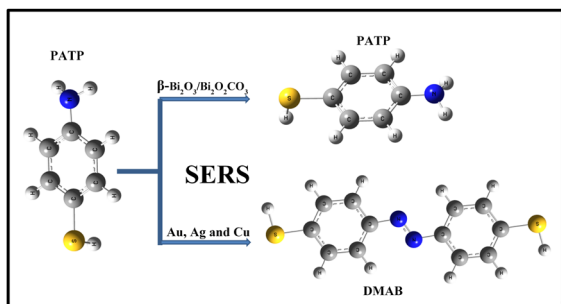
9559



Redox exfoliated NbS₂: characterization, stability, and oxidation

Danilo A. Nagaoka, Daniel Grasseschi, Alisson R. Cadore, Jessica E. S. Fonsaca, Ali M. Jawaid, Richard A. Vaia and Christiano J. S. de Matos*

9569



To dimerize or not: *para*-aminothiophenol on a bismuth heterostructure

Poonam Bhadoria, Arti Saroj and Venkatnarayan Ramanathan*

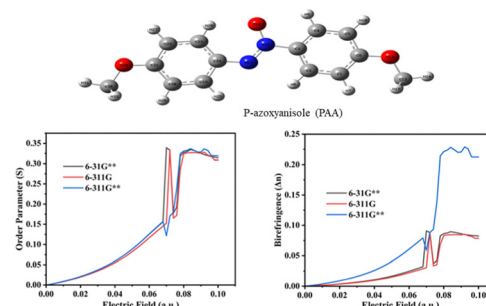


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9576

Quantum mechanical studies of *p*-azoxyanisole and identification of its electro-optic activity

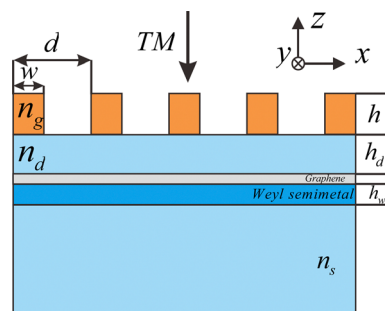
Manish Kumar, Mirtunjai Mishra, Devesh Kumar* and Devendra Singh*



9586

Tunable near-perfect nonreciprocal radiation with a Weyl semimetal and graphene

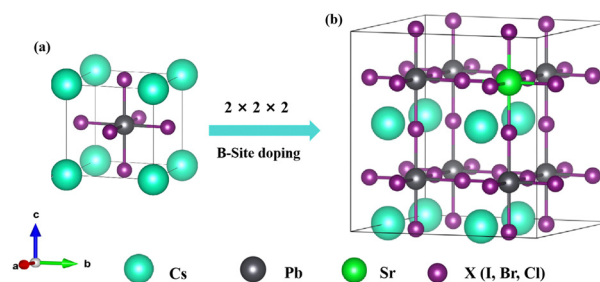
Jun Wu* and Ye Ming Qing*



9592

Influence of Sr doping on the photoelectronic properties of CsPbX₃ (X = Cl, Br, or I): a DFT investigation

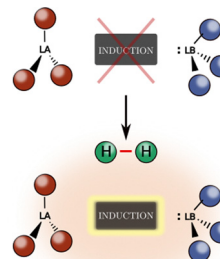
Man Zhang, Guangbiao Xiang, Yanwen Wu, Jing Liu, Jiancai Leng,* Chen Cheng* and Hong Ma*



9599

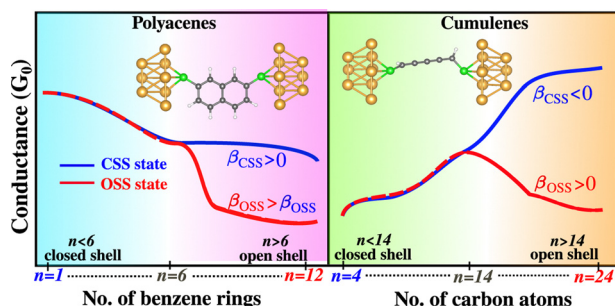
Three-body interaction effects in heterolytic hydrogen splitting by frustrated Lewis pairs

Małgorzata M. Szczeniak* and Grzegorz Chałasiński*



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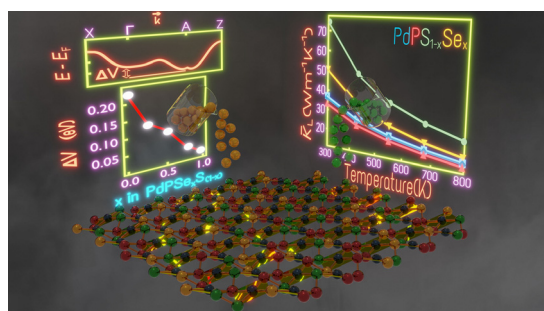
9607



Anti-ohmic nanoconductors: myth, reality and promise

Ashima Bajaj and Md. Ehesan Ali*

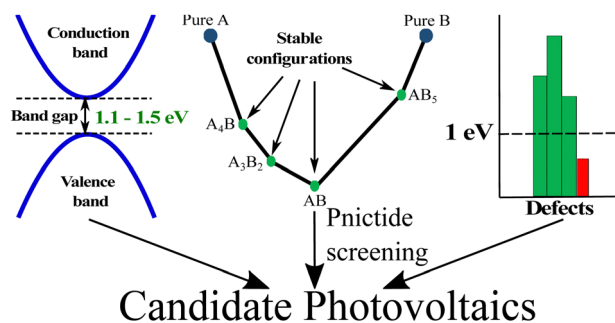
9617



Synergistic effect of alloying on thermoelectric properties of two-dimensional PdPQ (Q = S, Se)

S. Shahabfar, Y. Xia, M. H. Morshedsolouk, M. Mohammadi and S. Shahab Naghavi*

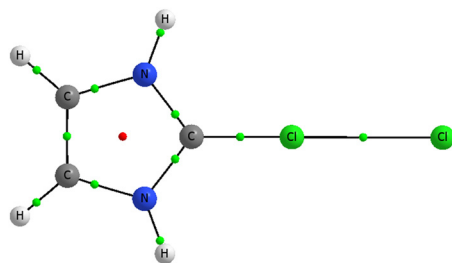
9626



Study of pnictides for photovoltaic applications

Jayant Kumar and Gopalakrishnan Sai Gautam*

9636

Complex of imidazol-2-ylidene with Cl₂

Halogen bonds with carbenes acting as Lewis base units: complexes of imidazol-2-ylidene: theoretical analysis and experimental evidence

Sławomir J. Grabowski

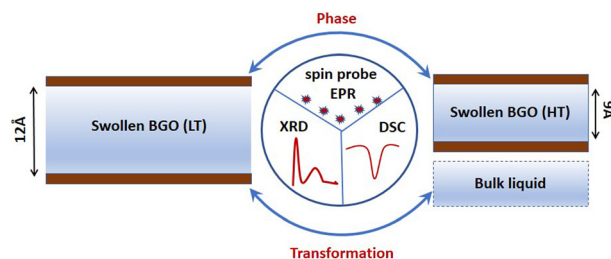


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9648

Phase transformation in the “Brodie graphite oxide–acetonitrile” system – influence of the oxidizing level of the material

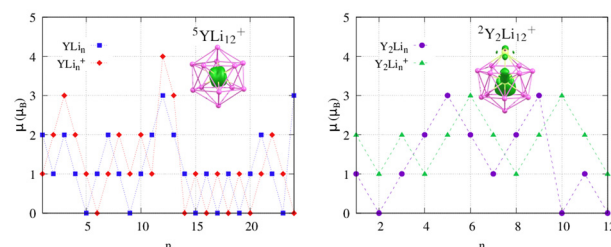
N. A. Chumakova,* D. S. Popov, A. V. Kaplin,
A. T. Rebrikova, E. A. Eremina, M. V. Korobov and
O. N. Khrykina



9656

On the energetic and magnetic stability of neutral and charged lithium clusters doped with one and two yttrium atoms

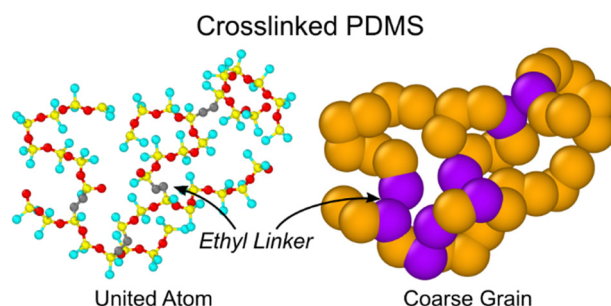
Henry Nicole González-Ramírez,* Héctor Xólotl Silos Vega,
Zeferino Gómez-Sandoval, Roberto Flores-Moreno,
Osvaldo Yáñez, Kayim Pineda-Urbina,
Juan Pablo Mojica-Sánchez and
José Manuel Flores-Álvarez



9669

United atom and coarse grained models for crosslinked polydimethylsiloxane with applications to the rheology of silicone fluids

Aditi Khot, Rebecca K. Lindsey, James P. Lewicki,
Amitesh Maiti, Nir Goldman and
Matthew P. Kroonblawd*



CORRECTION

9685

Correction: Noncovalent wedging effect catalyzed the *cis* to *syn* transformation of a surface-adsorbed polymer backbone toward an unusual thermodynamically stable supramolecular product

Zhi-Xuan Liu, Ling Yang, Yong-Gang Chen, Zhi-Yuan Tian and Zhi-Yong Yang*

