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Cover

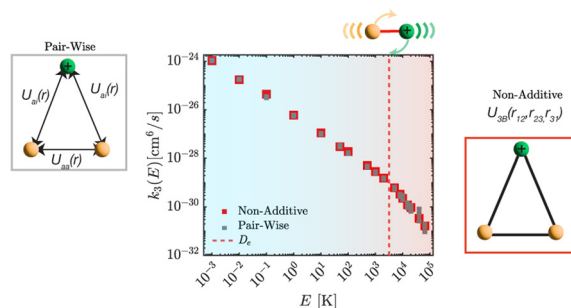
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COMMUNICATION

7264

On the role of non-additive interactions in three-body recombination

Yu Wang, Marjan Mirahmadi and Jesús Pérez-Ríos*

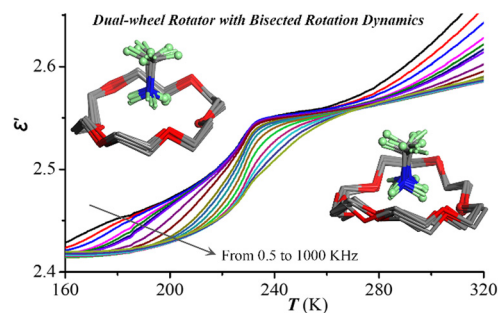


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A confinement-regulated ($\text{H}_3\text{C}-\text{NH}_3$)⁺ ion as a smallest dual-wheel rotator showing bisected rotation dynamics

Wang Li, Miao Xie, Shi-Yong Zhang, Cheng-Hui Zeng, Zi-Yi Du* and Chun-Ting He



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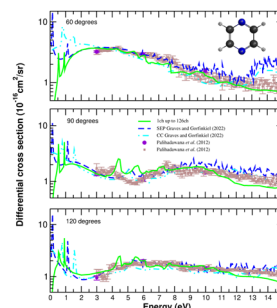


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Elastic and electronically inelastic scattering of electrons by the pyrazine molecule

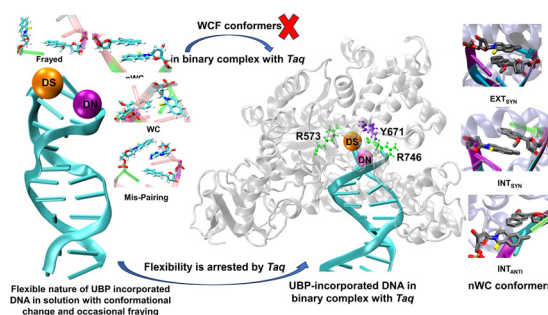
Murilo O. Silva,* Giseli M. Moreira, Jaime Rosado, Francisco Blanco, Gustavo García, Márcio H. F. Bettega and Romarly F. da Costa*



7287

Investigation of the stability of D5SIC-DNAM-incorporated DNA duplex in *Taq* polymerase binary system: a systematic classical MD approach

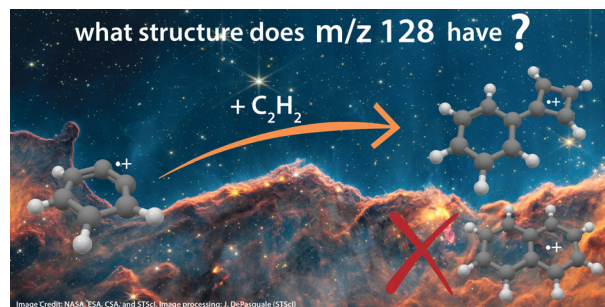
Tanay Debnath and G. Andrés Cisneros*



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Ionic fragmentation products of benzonitrile as important intermediates in the growth of polycyclic aromatic hydrocarbons

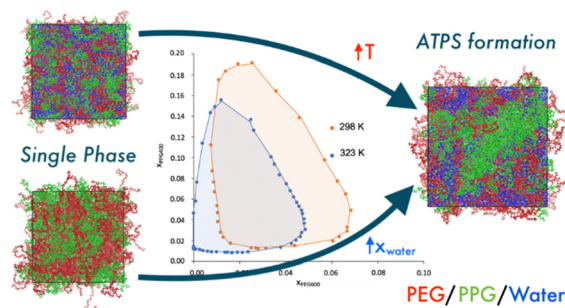
Daniël B. Rap, Johanna G. M. Schrauwen, Britta Redlich and Sandra Brünken*



7308

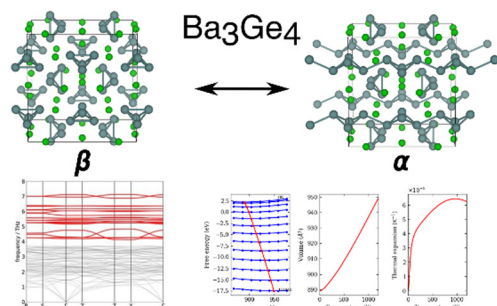
Unravelling the molecular interactions behind the formation of PEG/PPG aqueous two-phase systems

Alexandre M. S. Jorge, Gonalo M. C. Silva, João A. P. Coutinho* and Jorge F. B. Pereira*



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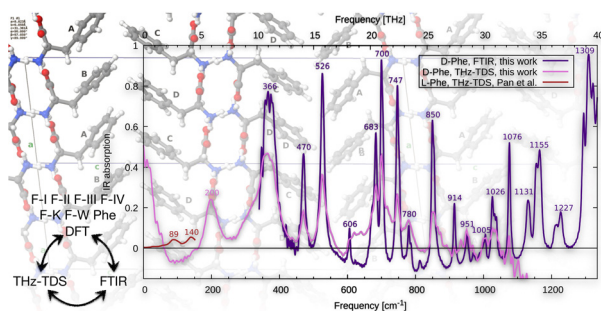
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Thermodynamics of phase transitions in Zintl clusters from density functional theory: making and breaking of bonds in Ba_3Ge_4

Yao Zhao and John E. McGrady*

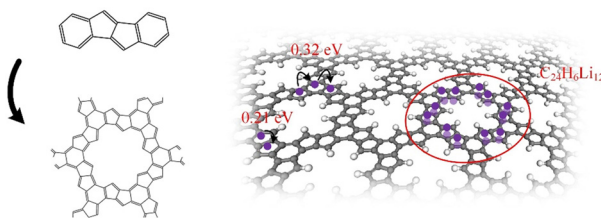
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THz to far-infrared spectra of the known crystal polymorphs of phenylalanine

Thomas A. Niehaus,* Emilien Prost, Vincent Lorient, Franck Lépine, Luc Bergé and Stefan Skupin

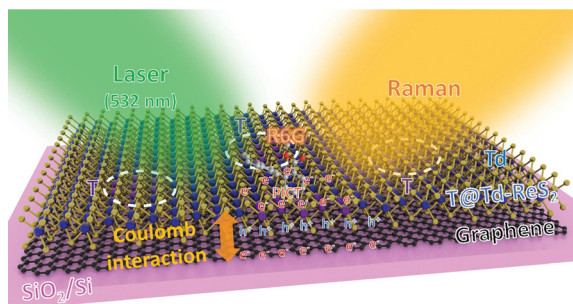
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Holey penta-hexagonal graphene: a promising anode material for Li-ion batteries

Linguo Lu, Raven Gallenstein, Xinghui Liu, Yi Lin, Shiru Lin* and Zhongfang Chen*

7343



Dynamic repulsive interaction enables an asymmetric electron-phonon coupling for improving Raman scattering

Jiawei Shen, Jiaxin Zhang, Zirui Fu, Yan Pan, Xiaowan Li, Shuyi Wu,* Yun Shan* and Lizhe Liu*

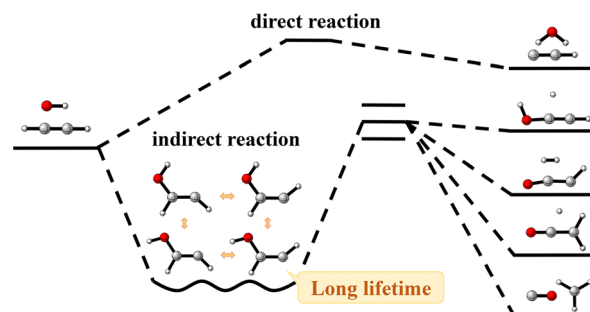


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Dynamics studies for the multi-well and multi-channel reaction of OH with C₂H₂ on a full-dimensional global potential energy surface

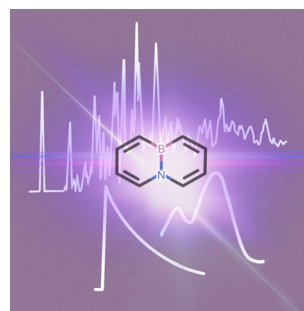
Shuwen Zhang, Qixin Chen, Lidong Zhang,* Jun Li,* Xixi Hu* and Daiqian Xie



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Impact of isoelectronic substitution on the excited state processes in polycyclic aromatic hydrocarbons: a joint experimental and theoretical study of 4a,8a-azaboranaphthalene

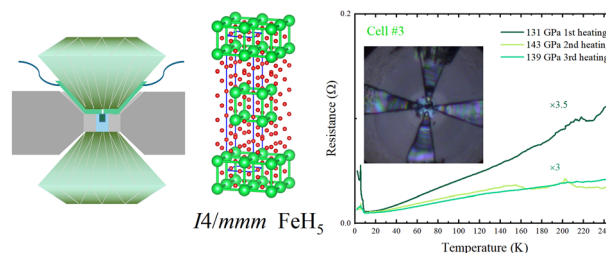
Floriane Sturm, Michael Bühler, Christoph Stapper, Johannes S. Schneider, Holger Helten, Ingo Fischer* and Merle I. S. Röhr*



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Absence of superconductivity in *I4/mmm*-FeH₅: experimental evidence

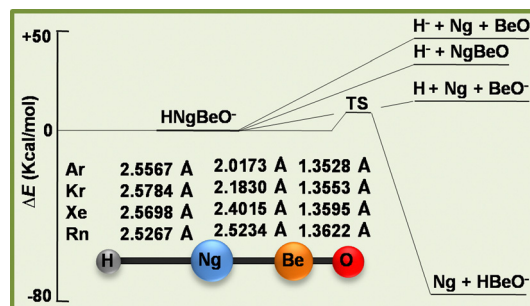
Yulong Wang, Su Chen, Jianning Guo, Xiaoli Huang* and Tian Cui



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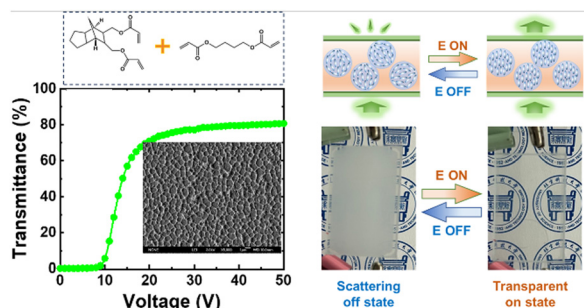
Noble gas hydrides: theoretical prediction of the first group of anionic species

Stefano Borocci, Patrizio Cecchi, Felice Grandinetti,* Nico Sanna and Costantino Zazza



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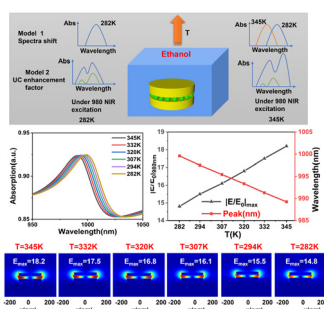
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Impact of crosslinking agents with steric cyclic groups on the properties of polymer-dispersed liquid crystals

Meina Yu, Xian He, Jing Qin, Yongchuan Hu, Qian Wang, Cheng Zou, Huiyun Wei, Xiao Wang,* Yanzi Gao* and Huai Yang*

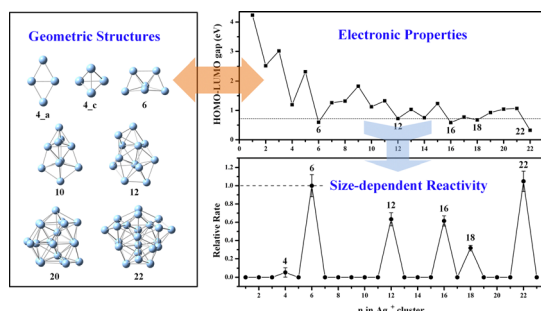
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Efficient monodisperse upconversion composite prepared using high-density local field and its dual-mode temperature sensing

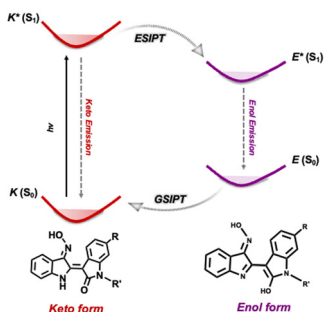
Huilin Li, Kai Zhao, Xiaoyan Liu, Shiping Zhan,* Guozheng Nie and Liang Peng

7407

Reactivity of cationic silver clusters with O₂: a probe of interplay between clusters' geometric and electronic structures

Jin Hu, Jun Ma, Zhengqian Jin, Wen Liu, Lulu Huang, Xuefeng Wang* and Xiaopeng Xing*

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The role of the oxime group in the excited state deactivation processes of indirubin

Daniela C. Nobre, Estefanía Delgado-Pinar, Carla Cunha and J. Sérgio Seixas de Melo*

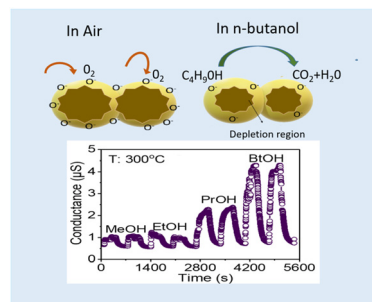


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Oxygen vacancy-enriched Zn_2SnO_4 for aliphatic alcohol sensing and enhanced selectivity towards *n*-butanol

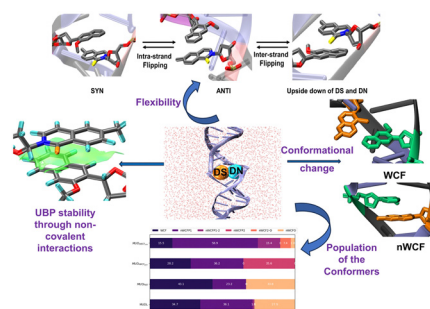
Reshmi Thekke Parayil, B. Bhagat, Santosh K. Gupta,*
K. Mukherjee* and Manoj Mohapatra



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Investigation of dynamical flexibility of D5SIC-DNAM inside DNA duplex in aqueous solution: a systematic classical MD approach

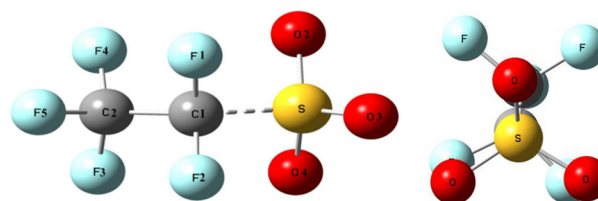
Tanay Debnath and G. Andrés Cisneros*



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Theoretical study on the degradation mechanism of perfluoro-ethanesulfonic acid under subcritical hydrothermal alkaline conditions

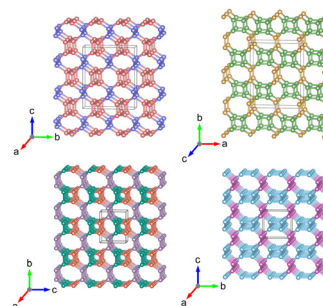
Lei Zhang, Zizhong Liu,* Ruisheng Zhao, Hua Zhao and Jian Wei



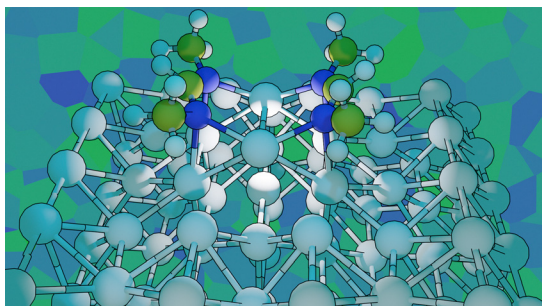
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Bottom-up design of carbon allotropes with tunable properties

Pan Ying, Yufei Gao,* Ziheng Li, Mengdong Ma, Chao Liu* and Guodong Tang*



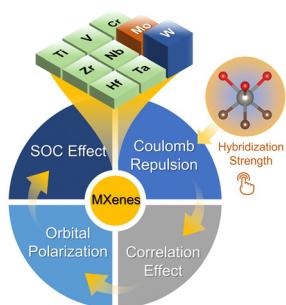
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Towards understanding the first half-ALD cycle of Ag growth: adsorption and dissociation of silver(I) acetaminidates on the Ag(110) surface

J. I. Paez-Ornelas,* Noboru Takeuchi and J. Guerrero-Sánchez

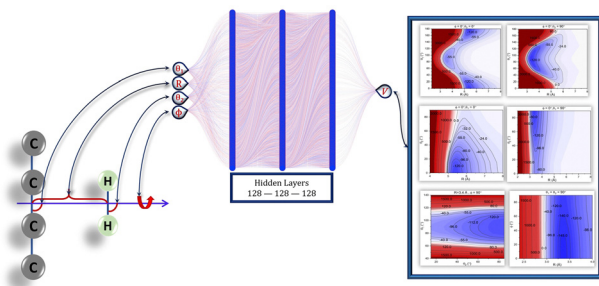
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Tuning d-orbitals to control spin-orbit coupling in terminated MXenes

Tao Yang,* Xiaojun Liu, Jian Fang, Zhi Liu, Zheng Qiao, Ziqiang Zhu, Qianju Cheng, Yaoyao Zhang* and Xiaolan Chen*

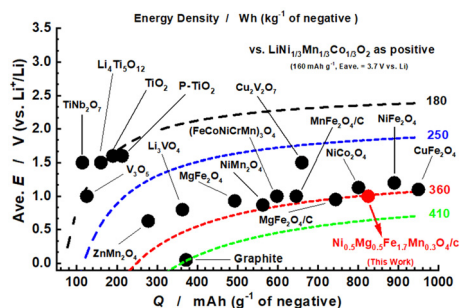
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Quantum rotational dynamics of $I-C_4(^3\Sigma_g^-)$ by H_2 at low temperatures employing a machine learning augmented potential energy surface

Pooja Chahal, Apoorv Kushwaha and T. J. Dhilip Kumar*

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Carbon-coated $Ni_{0.5}Mg_{0.5}Fe_{1.7}Mn_{0.3}O_4$ nanoparticles as a novel anode material for high energy density lithium-ion batteries

Khadija Kouchi, Marwa Tayoury, Abdelwahed Chari, Loubna Hdidou, Zakaria Chchiyai, Khadija El kamouny, Youssef Tamraoui, Bouchaib Manoun, Jones Alami and Mouad Dahbi*

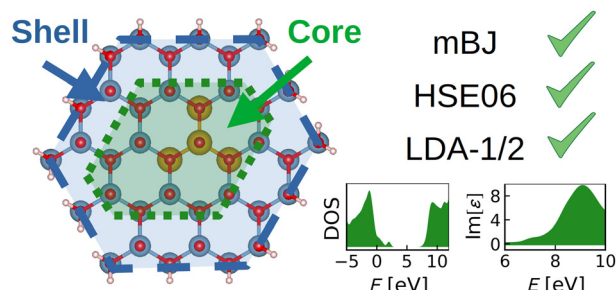


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Electronic and optical properties of core–shell InAlN nanorods: a comparative study *via* LDA, LDA-1/2, mBJ, HSE06, G_0W_0 and BSE methods

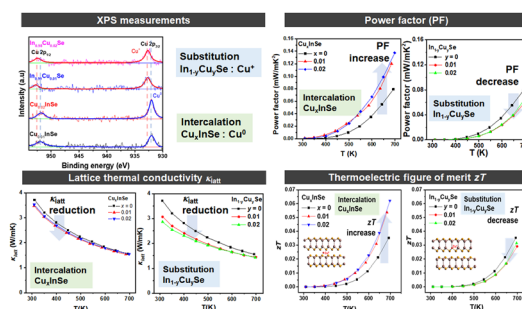
Ronaldo Rodrigues Pela,* Ching-Lien Hsiao,
Lars Hultman, Jens Birch and
Gueorgui Kostov Gueorguiev



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Comparison of influence of intercalation and substitution of Cu on electrical and thermoelectric transport properties of InSe alloys

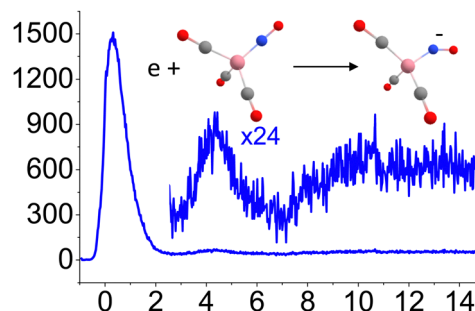
Hyungyu Cho, Jong Wook Roh, Sanghyun Park,
Seung Min Kang, Joontae Park and Sang-il Kim*



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Formation of negative ions from cobalt tricarbonyl nitrosyl $\text{Co}(\text{CO})_3\text{NO}$ clusters

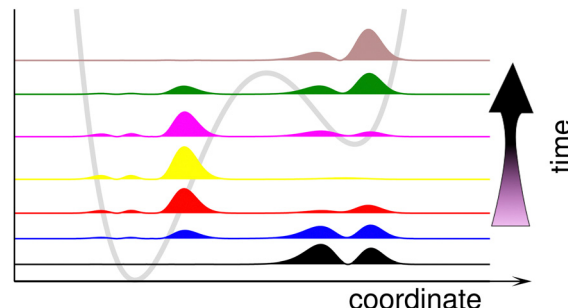
Dušan Mészáros, Štefan Matejčík and Peter Papp*



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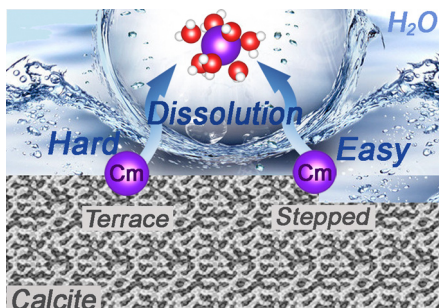
Coherent state switching using vibrational polaritons in an asymmetric double-well potential

Loïse Attal, Florent Calvo, Cyril Falvo and Pascal Parneix*



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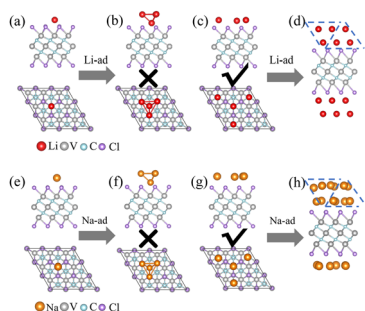
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Dynamic dissolution of Cm^{3+} ions incorporated at the calcite–water interface: an *ab initio* molecular dynamics simulation study

Zhao-Qin Chu, Ru-Yu Zhu and Jing Su*

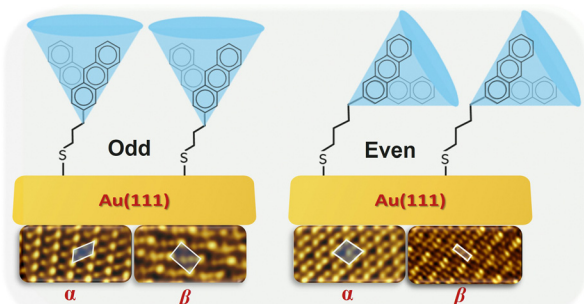
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Lattice matching and halogen regulation for synergistically induced large Li and Na storage by halogenated MXene $\text{V}_3\text{C}_2\text{Cl}_2$

Min Zhou, Yanqing Shen,* LingLing Lv, Yu Zhang, Xianghui Meng, Xin Yang, Qirui He, Bing Zhang, Long Pang,* Peng E* and Zhongxiang Zhou

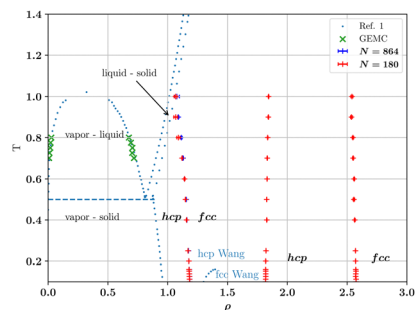
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Odd–even effects in aryl-substituted alkanethiolate SAMs: nonsymmetrical attachment of aryl unit and its impact on the SAM structure

Waleed Azzam,* Abdu Subaihi, Michael Rohwerder, Asif Bashir, Andreas Terfort* and Michael Zharnikov*

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Sensitivity of solid phase stability to the interparticle potential range: studies of a new Lennard-Jones like model

Olivia S. Moro,* Vincent Ballenegger, Tom L. Underwood and Nigel B. Wilding*

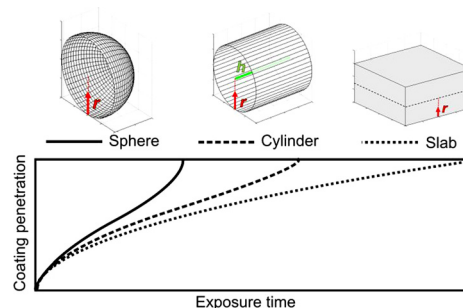


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An atomic layer deposition diffusion–reaction model for porous media with different particle geometries

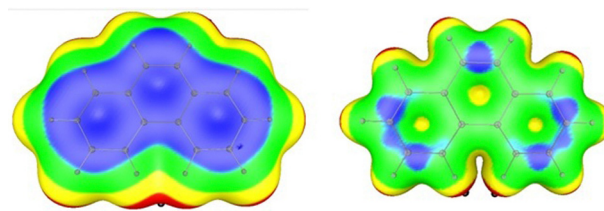
Niko Heikkinen,* Juha Lehtonen and Riikka L. Puurunen



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Probing intramolecular interactions using molecular electrostatic potentials: changing electron density contours to unveil both attractive and repulsive interactions

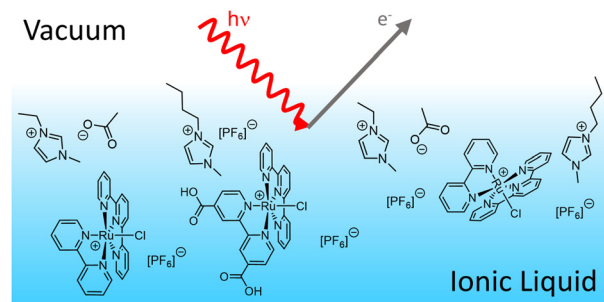
Goedele Roos and Jane S. Murray*



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Exploring the interfacial behavior of ruthenium complexes in ionic liquids: implications for supported ionic liquid phase catalysts

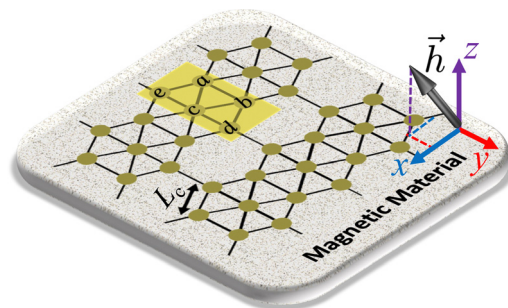
Daniel Hemmeter, Luciano Sanchez Merlinsky, Luis M. Baraldo, Florian Maier, Federico J. Williams* and Hans-Peter Steinrück*



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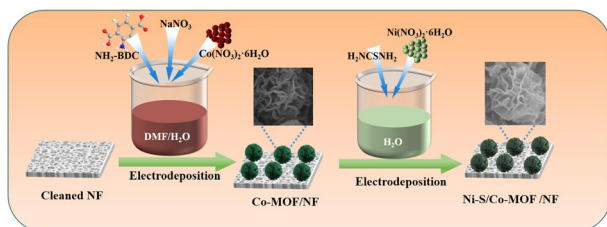
Substrate-induced strain and exchange field effects on the electronic and thermal properties of monolayer β_{12} -borophene

Bui Dinh Hoi, Le Thi Thu Phuong, Pham Viet Dung and Tran Cong Phong*



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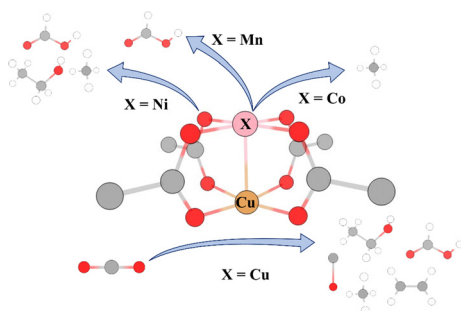
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Three-dimensional flower-like Ni-S/Co-MOF grown on Ni foam as a bifunctional electrocatalyst for efficient overall water splitting

Chang Su, Dan Wang, Wenchang Wang, Naotoshi Mitsuzaki, Rong Shao, Qi Xu and Zhidong Chen*

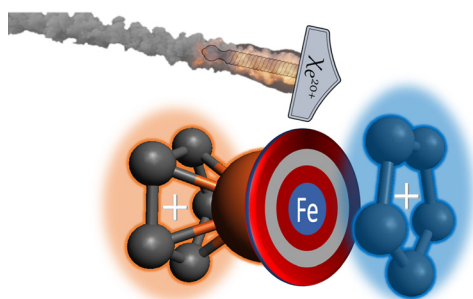
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Hetero-bimetallic paddlewheel complexes for enhanced CO₂ reduction selectivity in MOFs: a first principles study

Gavin A. McCarver,* Taner Yildirim and Wei Zhou

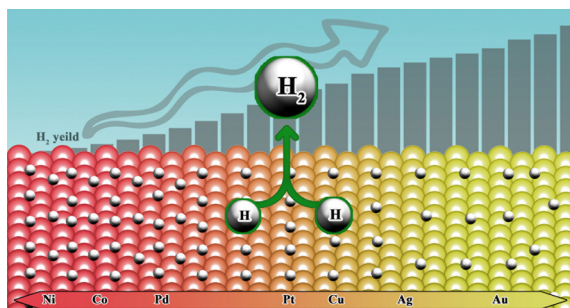
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Unexpected and delayed fragmentation dynamics of the organometallic ferrocene induced by ion-collision

F. Aguilar-Galindo, V. T. T. Nguyen, R. Singh, A. Domaracka, B. A. Huber, S. Díaz-Tendero, P. Rousseau and S. Maclot*

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Hydrogen adsorption on various transition metal (111) surfaces in water: a DFT forecast

Basil Raju Karimadom, Alina Sermiagin, Dan Meyerstein, Tomer Zidki, Amir Mizrahi, Ronen Bar-Ziv and Haya Kornweitz*

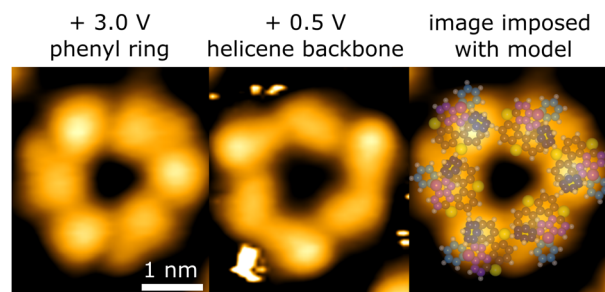


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STM/TERS observation of (*M*)-type diphenyl[7]thiaheterohelicene on Ag(111)

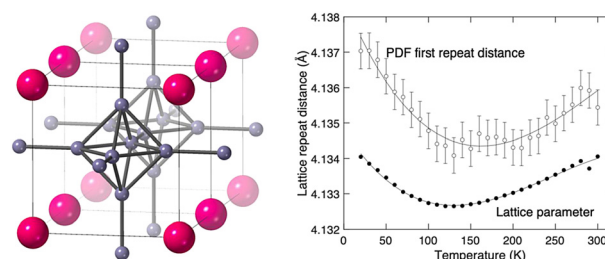
Sho Kimura, Takuma Hattori,* Changqing Ye, Masaki Okada, Satoshi Kondo, Yui Sakurama, Akira Saito, Pawel Krukowski, Hideji Osuga and Yuji Kuwahara



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Electronic origin of negative thermal expansion in samarium hexaboride revealed by X-ray diffraction and total scattering

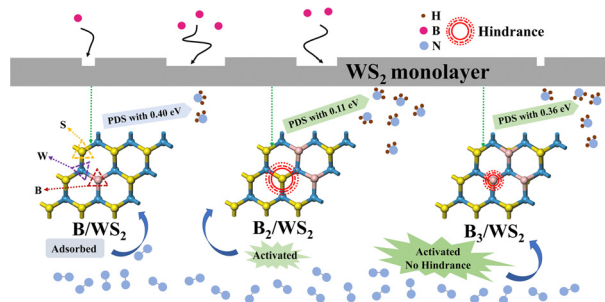
Li Li, Martin T. Dove,* Zhongsheng Wei, Anthony E. Phillips and Dean S. Keeble



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Computational investigation of single and multiple boron atom doped WS₂ monolayers for superior electrocatalytic reduction of nitrogen

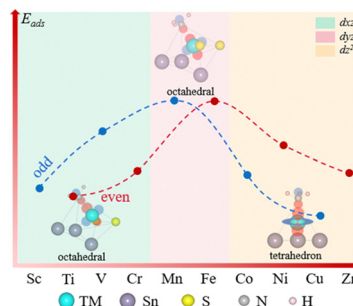
Zehong Yin, Jingeng Cao, Xiuyuan Li and Nan Li*



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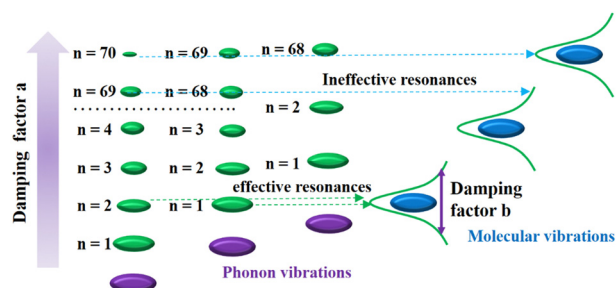
How spin state and oxidation number of transition metal atoms determine molecular adsorption: a first-principles case study for NH₃

Hua-Jian Tan, Rutong Si, Xi-Bo Li, Zhen-Kun Tang, Xiao-Lin Wei, Nicola Seriani,* Wen-Jin Yin* and Ralph Gebauer



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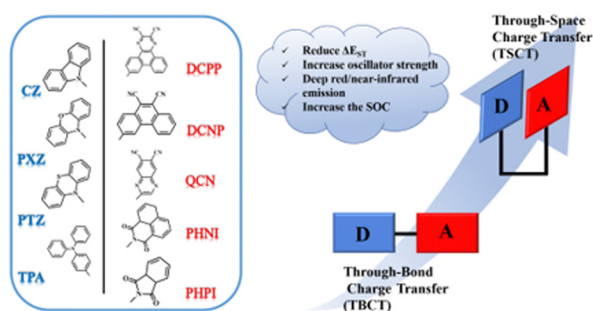
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Probing into the theory of impact sensitivity: propelling the understanding of phonon–vibron coupling coefficients

Wei-Hong Liu, Wei Zeng, Fu-Sheng Liu, Zheng-Tang Liu and Qi-Jun Liu*

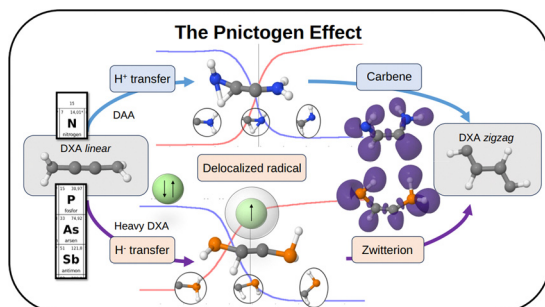
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Theoretical design and performance prediction of deep red/near-infrared thermally activated delayed fluorescence molecules with through space charge transfer

Xiaofang Li, Xiaofei Wang, Zhimin Wu, Kai Zhang, Rui Li, Yuzhi Song, Jianzhong Fan, Chuan-Kui Wang* and Lili Lin*

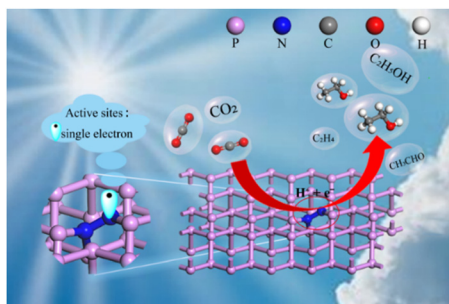
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Radical revelations: the pnictogen effect in linear acetylenes

Miguel Gallegos, Vicente del Amo, José Manuel Guevara-Vela, Guillermo Moreno-Alcántar and Ángel Martín Pendás*

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Efficient photoreduction of carbon dioxide to ethanol using diatomic nitrogen-doped black phosphorus

Jianhua Fan, Xin Wang,* Jing Ma, Xingman Liu, Xiaoyong Lai, Hongqiang Xia and Yingtao Liu*

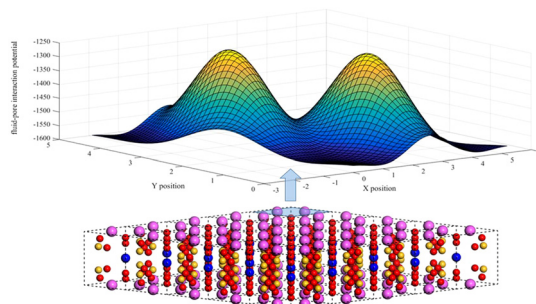


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Modeling carbon dioxide and methane adsorption on illite and calcite: enhancing the simplified local density model through crystal structure modifications

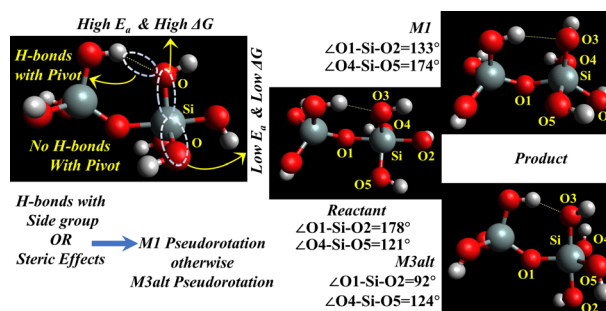
Gang Wu, Xiaofei Fu, Lu Wang, Rui Wang, Binhui Li and Zhejun Pan*



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Stereomutations in silicate oligomerization: the role of steric hindrance and intramolecular hydrogen bonding

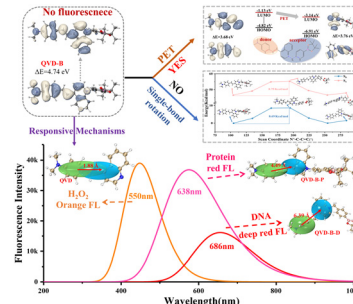
Dipak Prasad* and Nilanjan Mitra*



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Distinguishing the responsive mechanisms of fluorescent probes to hydrogen peroxide, proteins, and DNA/RNA

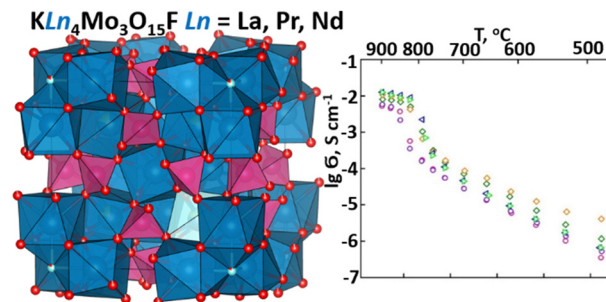
Lina Ding, Yang Liu, Liang Wang and Yonggang Yang*



7772

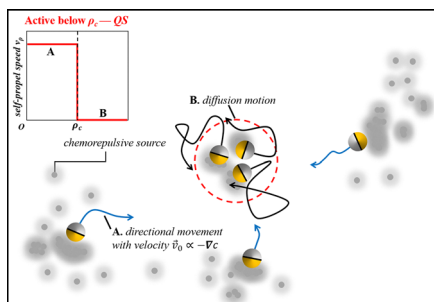
Extensive research of conductivity in the fluorite-like $\text{KLn}_4\text{Mo}_3\text{O}_{15}\text{F}$ ($\text{Ln} = \text{La, Pr, Nd}$) rare earth molybdates: theoretical and experimental data

Ekaterina I. Orlova,* Yelizaveta A. Morkhova,* Anastasia V. Egorova, Artem A. Kabanov, Egor D. Baldin, Elena P. Kharitonova, Nikolay V. Lyskov, Vasilii O. Yapaskurt, Olga A. Alekseeva, Valentina I. Voronkova and Daniil V. Korona



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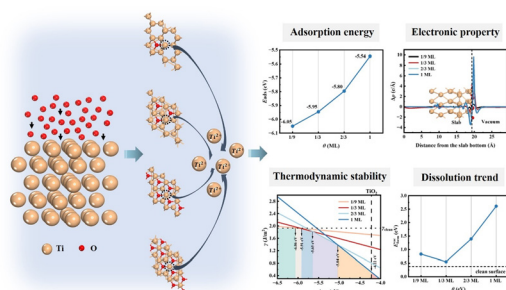
7783



Quorum sensing-induced transition from colloidal waves to Turing-like patterns in chemorepulsive active colloids

Jiaqi Cao, Jiaxin Wu and Zhonghuai Hou*

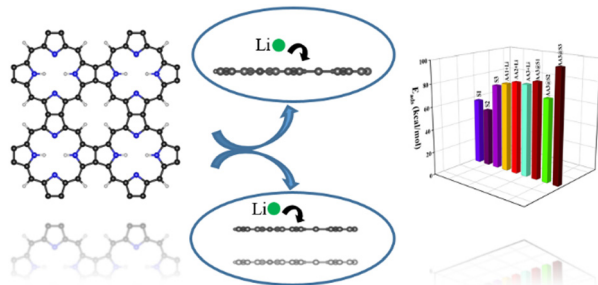
7794



Effects of oxygen adsorption on the corrosion behavior of the Ti(0001) surface: a DFT investigation

Xiaoting Wang, Dong Xie,* Huaiyuan Liu, Yantao Li, Fengjuan Jing and Yongxiang Leng*

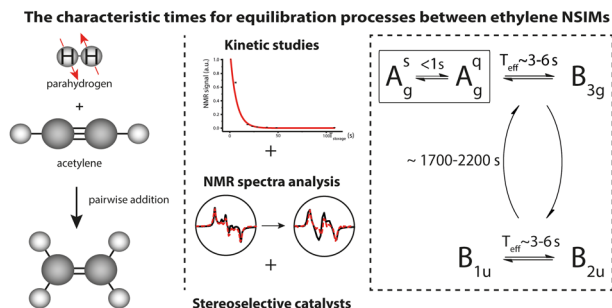
7808



Structural and electronic properties of Li-adsorbed single and bilayer porphyrin sheets as an electrode material for energy storage devices – a DFT analysis

Asnafarsin K. A., Anithaa V. S., Abhayram Balakrishnan, Rahul Suresh, Norge Cruz Hernandez and Vijayakumar Subramaniam*

7821



Manipulating stereoselectivity of parahydrogen addition to acetylene to unravel interconversion of ethylene nuclear spin isomers

Sergey V. Sviyazov, Simon V. Babenko, Ivan V. Skovpin, Larisa M. Kovtunova, Nikita V. Chukanov, Alexander Yu. Stakheev, Dudari B. Burueva* and Igor V. Koptug*

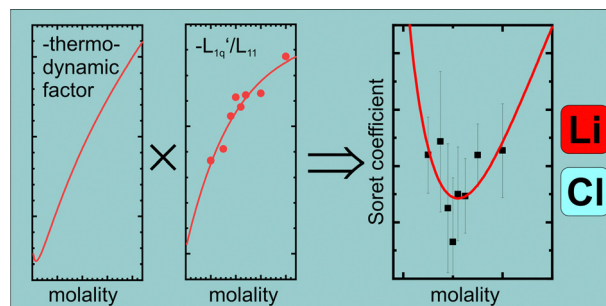


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7830

Non-monotonic Soret coefficients of aqueous LiCl solutions with varying concentrations

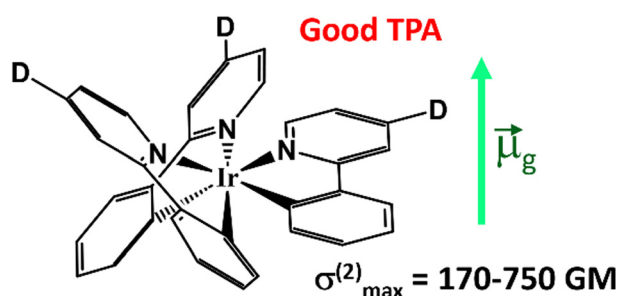
Namkyu Lee, Shilpa Mohanakumar, W. J. Briels* and Simone Wiegand*



7837

Two-photon absorption properties of simple neutral Ir(III) complexes

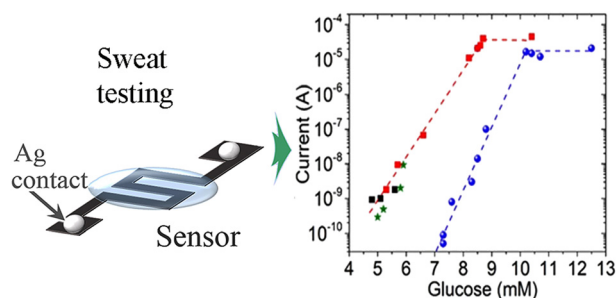
Eleonora Garoni, Alessia Colombo, Dominique Roberto, Claudia Dragonetti,* Veronique Guerschais and Kenji Kamada*



7844

Engineering of graphene-based composites with hexagonal boron nitride and PEDOT:PSS for sensing applications

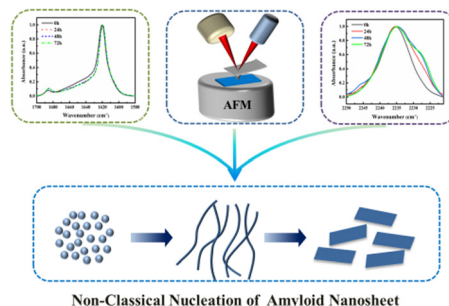
Irina V. Antonova,* Artem I. Ivanov, Marina B. Shavelkina, Dmitriy A. Poteryayev, Anna A. Buzmakova and Regina A. Soots



7855

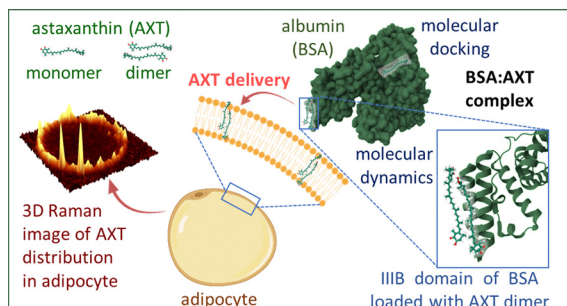
Unravelling the non-classical nucleation mechanism of an amyloid nanosheet through atomic force microscopy and an infrared probe technique

Yao Wang, Ziqi Wang, Lujuan Yang, Wenkai Zhang* and Gang Ma*



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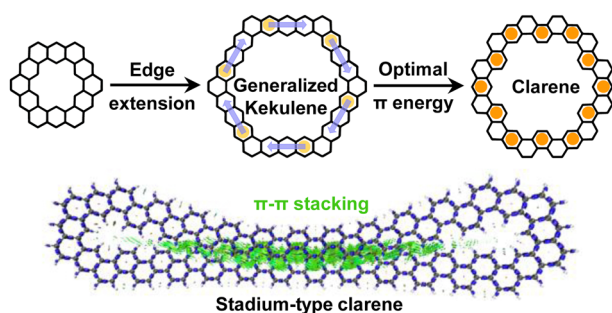
7865



Efficient delivery of carotenoids to adipocytes with albumin

Joanna Mazurkiewicz, Ewa Stanek, Aleksandra Kolodziejczyk, Marta Karpiel, Krzysztof Czamara, Tiago H. Ferreira, Pedro Maximiano, Pedro N. Simões, Igor Reva, Justyna Kalinowska-Tłuścik and Agnieszka Kaczor*

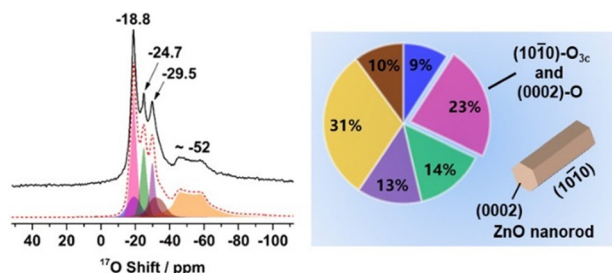
7877



Generalized kekulenes and clarenes as novel families of cycloarenes: structures, stability, and spectroscopic properties

Ke Du and Yang Wang*

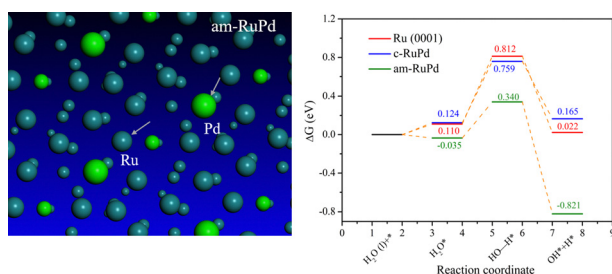
7890



^{17}O solid-state NMR study on exposed facets of ZnO nanorods with different aspect ratios

Benteng Song,* Yuhong Li, Yunhua Sun, Luming Peng and Ling-Hai Xie*

7896



Amorphous RuPd bimetallic for hydrogen evolution reaction in acidic and alkaline conditions: a first-principles study

Manman Liu, Xiaofeng Fan,* Xiaoqiang Cui, Weitao Zheng and David J. Singh

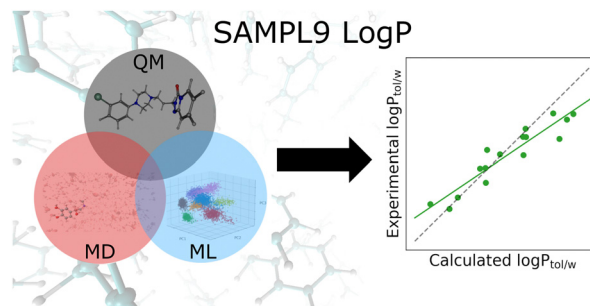


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Integrating multiscale and machine learning approaches towards the SAMPL9 log *P* challenge

Michael R. Draper, Asa Waterman, IV,
Jonathan E. Dannatt* and Prajay Patel*



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The crucial role of transient tri-coordinated oxygen in the flow of silicate melts

Longfei Gao, Xingchen Liu,* Jin Bai,* Bo Chen, Min Wu,
Lingxue Kong, Zongqing Bai and Wen Li

