

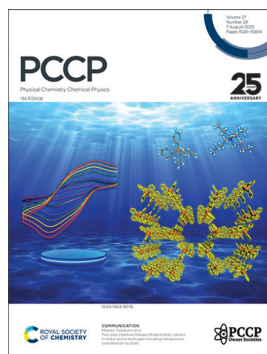
IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 27(29) 15241–15804 (2025)



Cover

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Inside cover

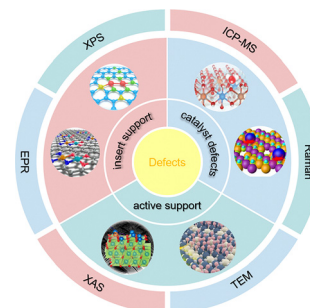
See Makoto Tadokoro *et al.*, pp. 15310–15313. Image reproduced by permission of Makoto Tadokoro from *Phys. Chem. Chem. Phys.*, 2025, 27, 15310.

REVIEWS

15256

Atomic vacancy defect-induced dual active sites synergistic catalysis for oxygen evolution reaction

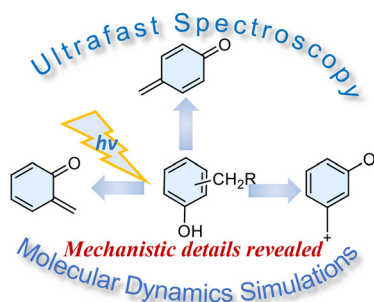
Zhenwen Yu, Yong Gao, Xueping Hong, Miaoxia Ji and Kun Chang*



15272

Mechanistic investigations of photochemical generation of quinone methides

Lingfeng Ge, Yan Guo, Shu-Lin Zhang, David Lee Phillips, Nikola Basarić* and Jiani Ma*



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15293

Recent advances in lasing phenomena in cholesteric liquid crystals: materials, mechanisms and applications

Aneela Ahmad, Haitao Dai,* Shouzhong Feng, Minxuan Li, Darakhshan Mehvish, Zolkefl Mohmaed, Samia Arain and Zhenda Chen

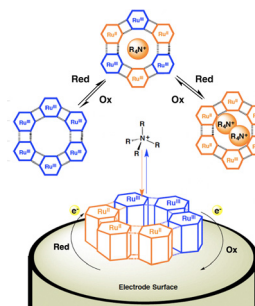


COMMUNICATION

15310

Two-step insertion/release of electrolytic cations in redox-active hydrogen-bonding nanoporous coordination crystals

Makoto Tadokoro,* Ryota Nishimura, Hajime Kamebuchi, Fumiya Kobayashi, Jun Miyazaki and Masa-aki Haga

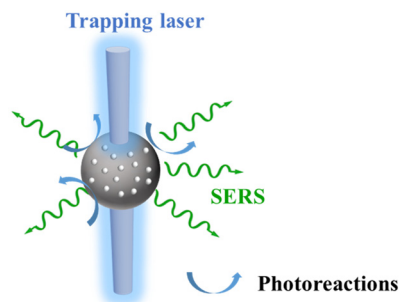


RESEARCH PAPERS

15314

Probing photoreactions of individual suspended carbonaceous aerosols by multi-wavelength OT-SERS

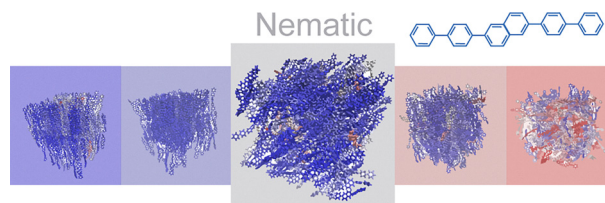
Hang Zhong, Jun Chen,* Yi Hu, Jun Chen, Tao Shao and Junsheng Liao*



15321

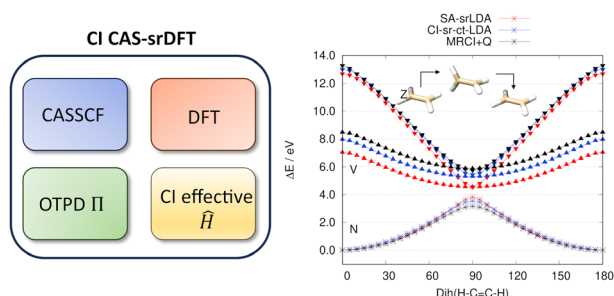
Insights into the nanostructuring and phase behaviour of an all-aromatic prototypical nematic liquid crystal

Henry Adenusi,* Luca Muccioli, Matteo Lanciotti, Maruti Hegde, Theo J. Dingemans, Edward T. Samulski, Francesco Vita and Oriano Francescangeli*



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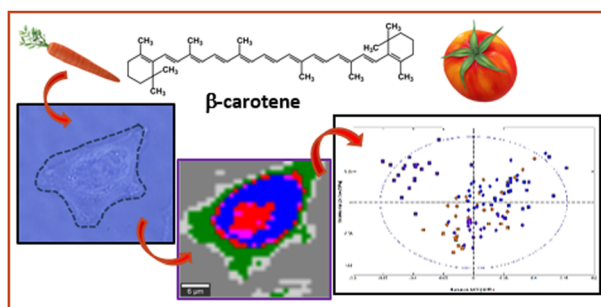
15331



Excited-state methods based on state-averaged long-range CASSCF short-range DFT

Benjamin Helmich-Paris,* Erik Rosendahl Kjellgren and Hans Jørgen Aa. Jensen

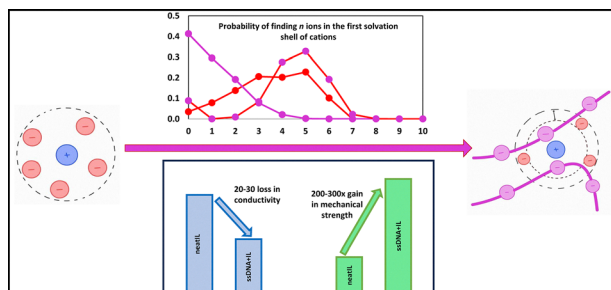
15350



In vitro analysis of β -carotene supplementation: insights from Raman spectroscopy on brain, lung, and breast cancer cells

Karolina Jarczewska, Monika Kopeć and Jakub Maciej Surmacki*

15367

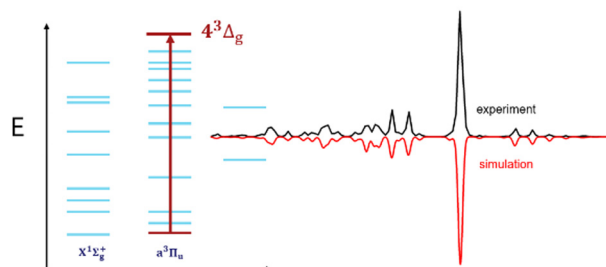


Molecular simulations of ssDNA/ssRNA in [BMIM][PF₆] ionic liquid: a novel biopolymer electrolyte for rechargeable battery applications

Akash K. Meel and Santosh Mogurampelly*

15376

Highest experimentally identified state of C₂



Experimental identification of the high-lying $4^3\Delta_g$ state of C₂ in the vacuum ultraviolet region

Di Li, Liying Ma, Tonghui Yin, Pan Jiang, Min Cheng* and Hong Gao*

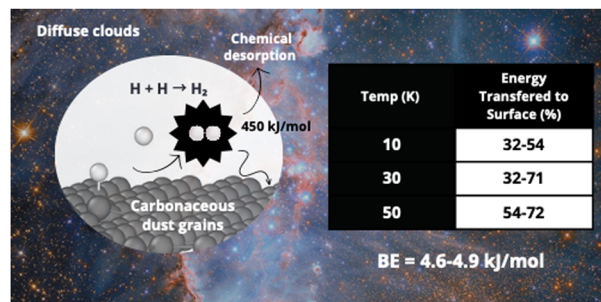


RESEARCH PAPERS

15385

Energy partitioning in H_2 formation on interstellar carbonaceous grains. Insights from *ab initio* molecular dynamics simulations

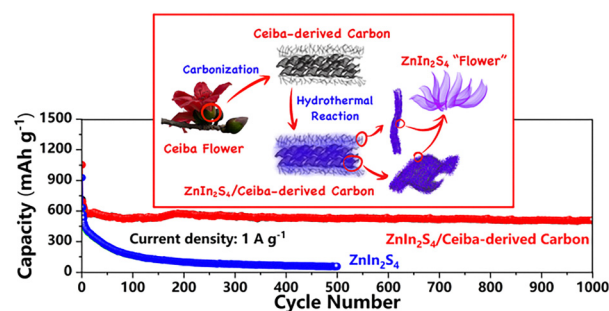
Léana Jubert, Berta Martínez-Bachs, Gerard Pareras and Albert Rimola*



15398

Ceiba flower-derived hard carbon with multi-dimensional self-supported structures and its $ZnIn_2S_4$ -based composites: long-term stable anode materials for sodium-ion batteries

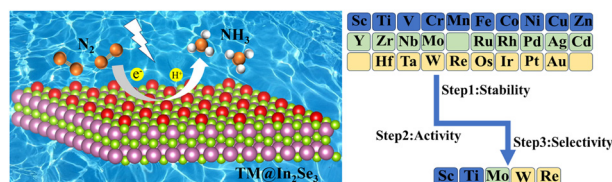
Xiaoyu Wu,* Wenting Liu, Zhenzhen Wu and Feng Lin



15407

Tunable electrocatalytic nitrogen reduction reactions via polarization switching on In_2Se_3 -based single-atom catalysts

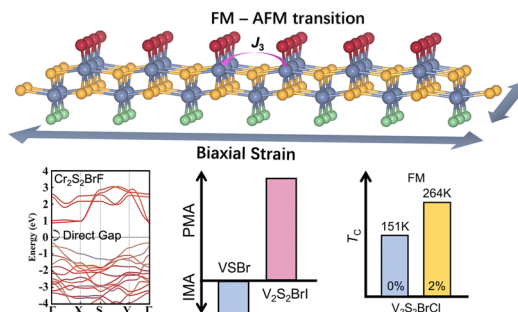
Huifang Wu, Linrui Zhao and Yukai An*



15417

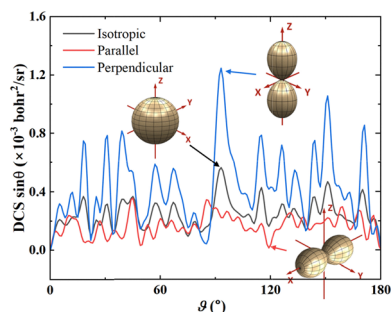
Tunable magnetic anisotropy and phase transitions in 2D Janus transition-metal chalcogenide halides

Siyu Han, Jiaqi Wang, Tong Zhao, Jian Zhou, Naihua Miao* and Zhimei Sun*



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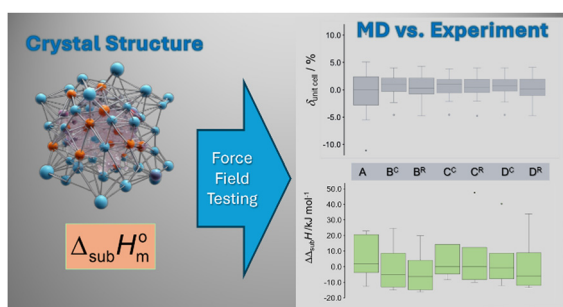
15427



Quantum stereodynamics of the $\text{Na}(^2\text{S}) + \text{NaLi}(X^1\Sigma^+) \rightarrow \text{Li}(^2\text{S}) + \text{Na}_2(X^1\Sigma_g^+)$ reaction: effect of NaLi molecular alignment

Hanghang Chen, He Huang and Maodu Chen*

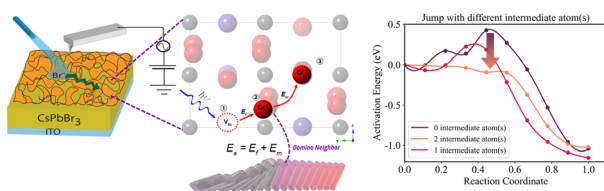
15435



An all-atom force field for MD simulations on organosulfur and organohalogen active pharmaceutical ingredients developed from experimental sublimation enthalpies and single crystal X-ray diffraction data

Cátia S. D. Lopes, Manuel E. Minas da Piedade and Carlos E. S. Bernardes*

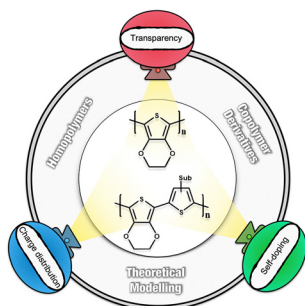
15446



Low-energy pathways lead to self-healing defects in CsPbBr_3

Kumar Miskin,* Yi Cao, Madaline Marland, Farhan Shaikh, David T. Moore, John A. Marohn and Paulette Clancy

15460



Computational study of PEDOT derivatives: reducing air stability to satisfy the self-doping criteria of transparent conjugated polymers

Florian Regnier, Mario Leclerc* and Jérôme Cornil*

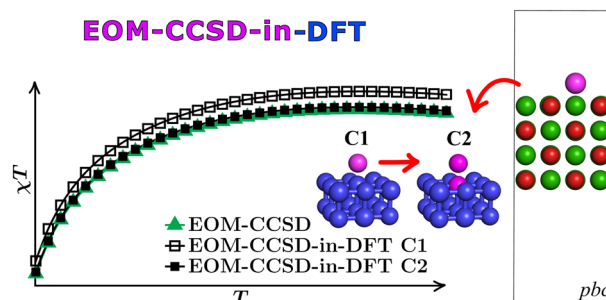


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15474

Quantum-embedded equation-of-motion coupled-cluster approach to single-atom magnets on surfaces

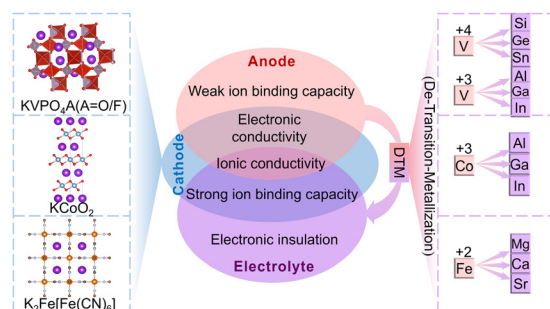
Maristella Alessio,* Tobias Schäfer, Thomas-C. Jagau and Andreas Grüneis



15486

De-transition-metallization of cathode materials for constructing high-performance solid-state electrolytes in potassium-ion batteries

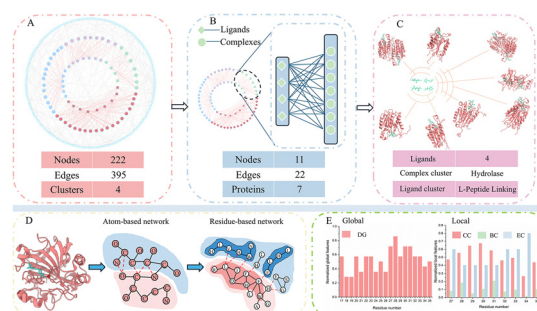
Mengqi Wu, Meitong Liu, Xiangyu Yao, Chenyang Jing, Dongxiao Kan* and Ruqian Lian*



15495

A multi-scale perspective on the scale-free nature of protein–ligand interaction networks

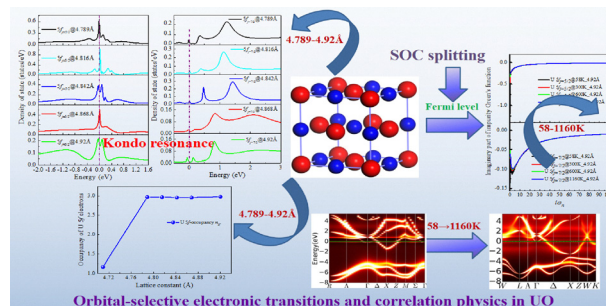
Zhongyi Wei, Chengwei Zeng, Chen Zhuo, Haoquan Liu, Jiaming Gao, Yuqing Zhao and Yunjie Zhao*



15508

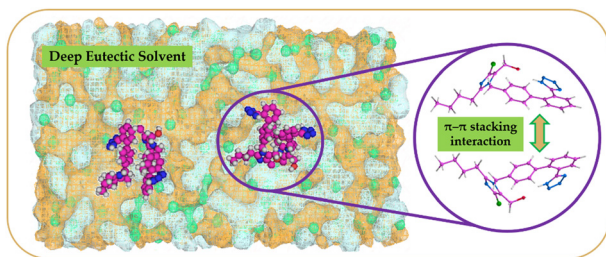
Spin–orbit-controlled correlation physics and orbital-selective electronic transitions in uranium monoxide revealed by many-body calculations

Ru-song Li,* Rong Guo,* Zheng Xie, Jin-tao Wang and Fei Wang



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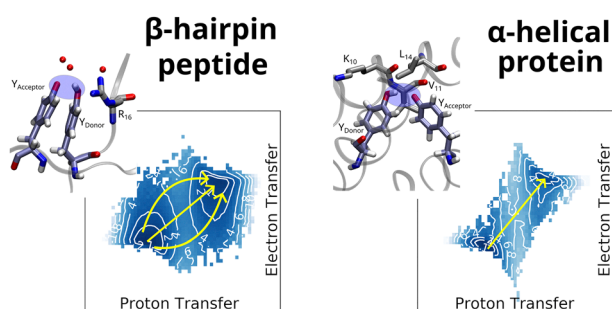
15527



Solvation and aggregation of heteroaromatic drugs in the Reline deep eutectic solvent – a combined molecular dynamics simulation and DFT study

Narges Karimi, Maryam Heydari Dokoohaki, Amin Reza Zolghadr* and Axel Klein*

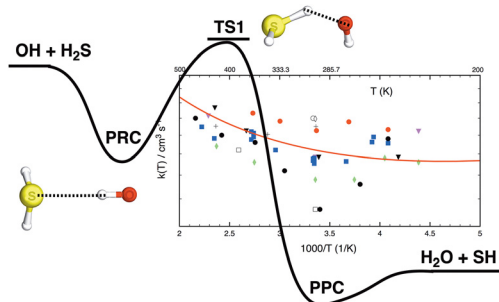
15544



Structural and environmental effects on the mechanism of biological proton-coupled electron transfer using DFTB/MM metadynamics

Katharina Spies, Leonie Pfeffer, Tomáš Kubař* and Natacha Gillet*

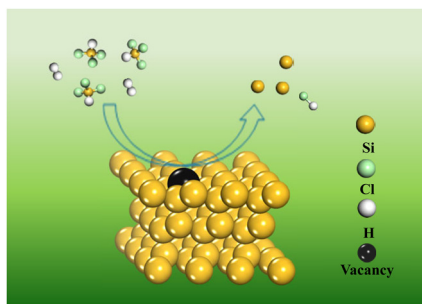
15557



High-accuracy theoretical rate coefficients for the reaction of H₂S with OH

Thanh Lam Nguyen,* Jozef Peeters* and John F. Stanton*

15566



Revealing the role of Si vacancies and interfaces in SiHCl₃ dissociation applied in polysilicon

Mao Peng, Jia Ren, Wei Li, Chenliang Ye* and Jinli Zhang*

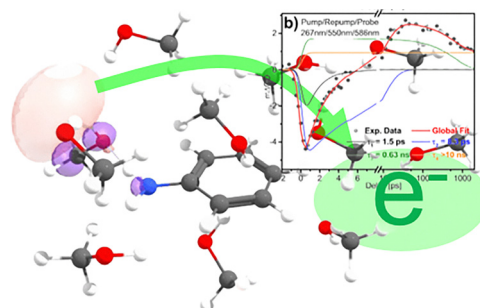


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15574

Relaxation dynamics of aniline in methanol: the photoionization channel

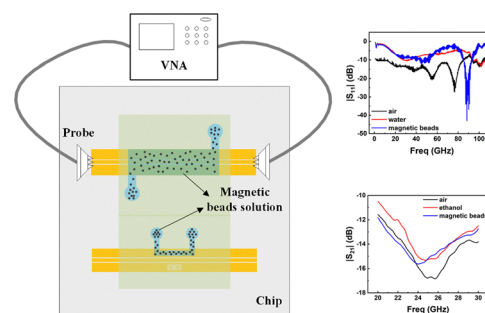
Raúl Montero, Iker Lamas, Marta Fernández-Fernández, Andrew W. Prentice, Dave Townsend, Martin J. Paterson and Asier Longarte*



15584

Microwave microfluidic sensors for analyzing magnetic bead-based bioliquids: from theory to experimental validation

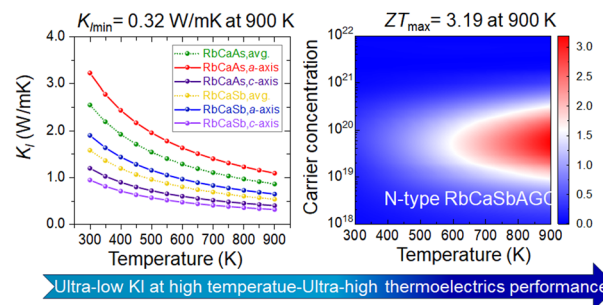
Linxiang Shao, Xiue Bao,* Zhaoying Li, Chaoran Xing, Giovanni Crupi, Giovanni Gugliandolo, Mariangela Latino, Liming Si, Houjun Sun and Lianggong Wen



15594

Low lattice thermal conductivity induced by rattling-like vibration in RbCaX (X = As, Sb) compounds with excellent thermoelectric properties

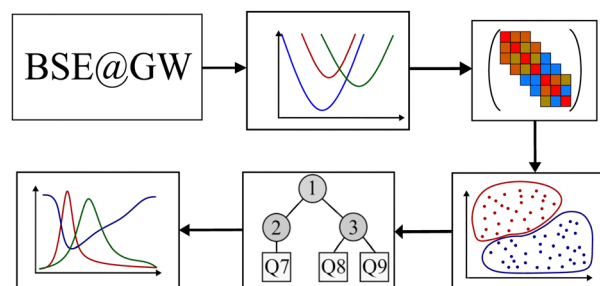
Jingyi Zhang, Junhao Peng, Runqing Zhang, Yanwei Liang, Zihan Xu, Renhai Wang, Fugen Wu,* Da Wan, Pengfei Zhang, Shulin Bai and Huafeng Dong*



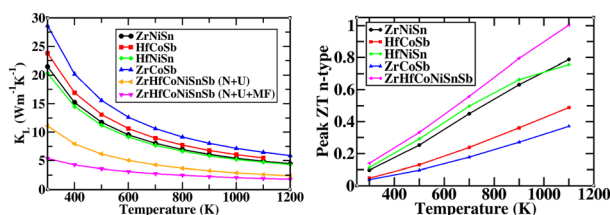
15609

BSE@GW-based protocol for spin-vibronic quantum dynamics using the linear vibronic coupling model. Formulation and application to an Fe(II) compound

Florian Bogdajn, Sebastian Mai, Leticia González and Oliver Kühn*



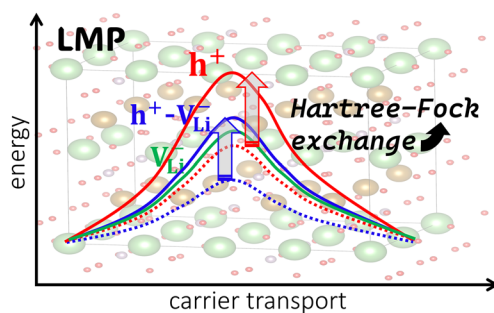
15622



Entropy-stabilized ZrHfCoNiSnSb half-Heusler alloy for thermoelectric applications: a theoretical prediction

Rajeev Ranjan

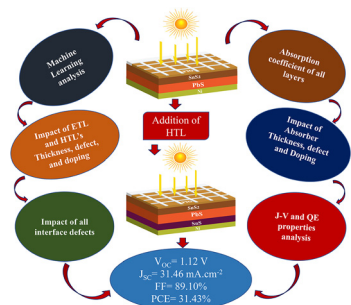
15635



A systematic study on carrier transport processes in charging olivine phosphates LiMPO₄ (M = Fe and Mn) by hybrid DFT calculations

Hiroshi Nakano and Hisao Nakamura*

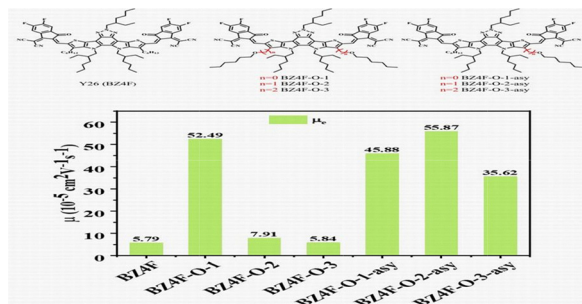
15645



Enhancement of sulfide-based absorber and charge transport layer solar cell performance using machine learning and the SCAPS-1D simulator

Avijit Ghosh,* Nondon Lal Dey, Mahbuba Moumita, Md. Jakaria Talukder, Abrar Ahamed Habibullah, Ripan Kumar Prodhan, Md. Towfiq uz zaman, Md. Majharul Islam, Aijaz Rasool Chaudhry and Md. Aktarujjaman

15669



Asymmetric alkoxy side chain engineering on A-DA'D-A non-fullerene acceptors: an effective strategy to enhance crystallinity and electron mobility

Wencheng Li, Zhijun Cao, Xingyu Xie, Yingping Zou* and Shaohui Zheng*

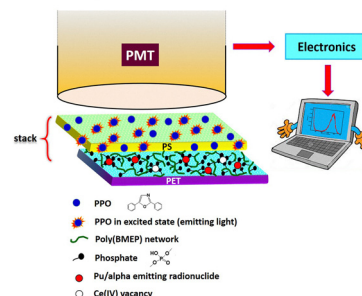


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15680

Imprinted polyethylene terephthalate: novel plutonium-selective substrates for ultra-trace detection

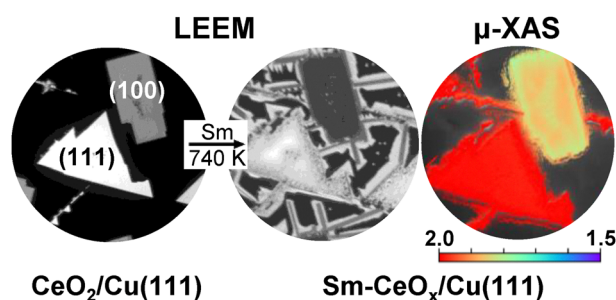
Amol Mhatre, Chhavi Agarwal,* Arunasis Bhattacharyya and Rahul Tripathi*



15691

The relationship between Sm alloying and structure sensitivity of ceria(111)- and (100)-oriented nanoislands on Cu(111)

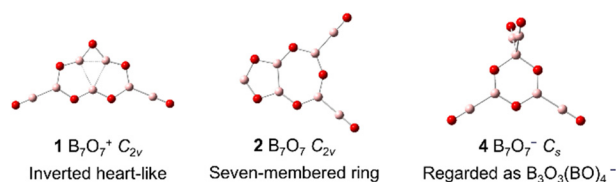
Emilia Pożarowska, Linus Pleines, Mauricio J. Prieto, Liviu C. Tănase, Lucas de Souza Caldas, Aarti Tiwari, Thomas Schmidt, Jens Falta, Carlos Morales and Jan Ingo Flege*



15704

Structural diversity in $B_7O_7^{+/0/-}$ clusters: emergence of a seven-membered ring and an inverted heart-like ring stabilized by 3c–2e localized bonds

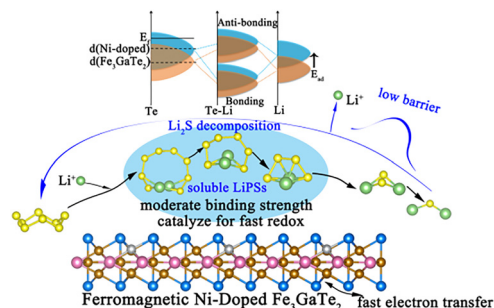
Wen-Juan Tian,* Zi-Yan Guo, Jing-Jing Wang, Hui-Qing Sun, Feng-Li Yang, Rui Bao and Hong-Xin Lv



15714

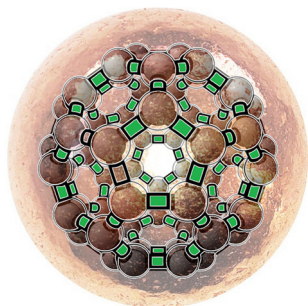
Ferromagnetic two-dimensional Fe_3GaTe_2 and Ni-doped Fe_3GaTe_2 as electrocatalysts for lithium–sulfur batteries: a first-principles study

Junru Wang,* Zhichao Liu, Yinchang Zhao* and Zhenhong Dai*



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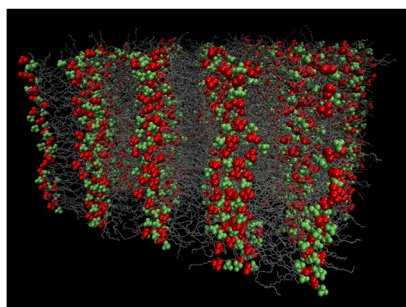
15723



Coating the fullerene: evaluation of the core–shell interaction nature in a saturated exohedral cuprofullerene

Raul Guajardo-Maturana, Carlos Rivera, Peter L. Rodríguez-Kessler and Alvaro Muñoz-Castro*

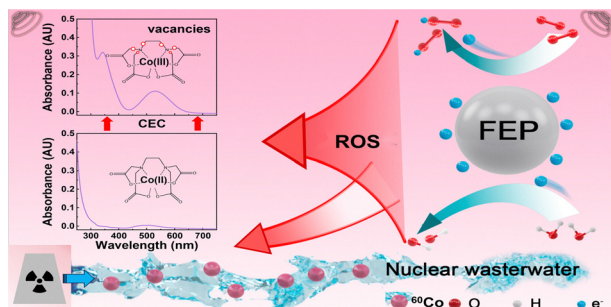
15731



Molecular dynamics simulations of discotic ionic liquid crystals: comparison of a full-charge and a scaled-charge force field

Valerio Mazzilli and Giacomo Saielli*

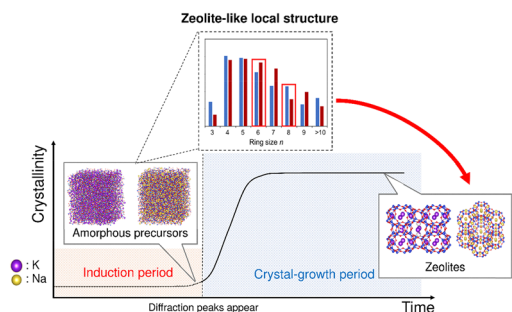
15742



Promoting Co(II)–EDTA decomplexation by central atom oxidation in contact-electro-catalysis

Zhenyi Chen, Shuo Li, Kun Feng,* Zhen Wen* and Jun Zhong*

15749



Influence of alkali metal cations on the local structure of amorphous precursors during zeolite crystallization

Kazuki Mori, Peidong Hu, Kentaro Kobayashi, Hiroki Yamada, Koji Ohara, Yutaka Yanaba, Tatsuya Okubo and Toru Wakihara*

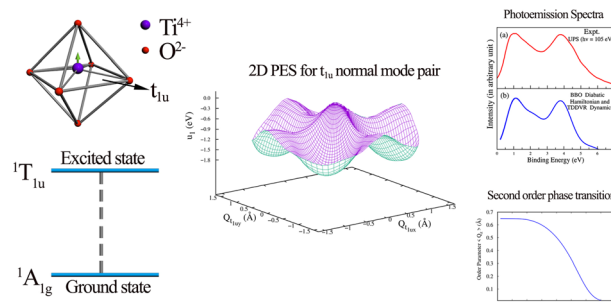


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15759

Construction of first-principles-based adiabatic and diabatic Hamiltonians for the TiO_6^{8-} unit of the BaTiO_3 crystal: photoemission spectra and ferroelectricity

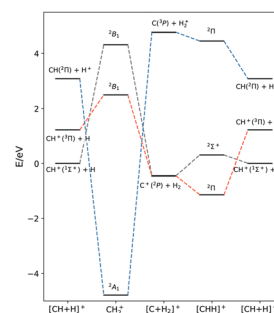
Mantu Kumar Sah, Soumya Mukherjee, Satyam Ravi and Satrajit Adhikari*



15775

Understanding the destruction of CH^+ with atomic hydrogen at low temperatures: a non-adiabatic dynamical study

Pablo del Mazo-Sevillano, Alfredo Aguado, François Lique, Rafael A. Jara-Toro and Octavio Roncero*



15787

Theoretical analysis of the Norrish reaction mechanism in aliphatic polyamide

Jingcheng Sang, Yuuichi Orimoto and Yuriko Aoki*

