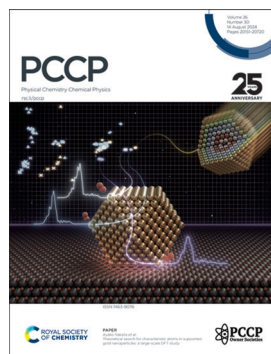


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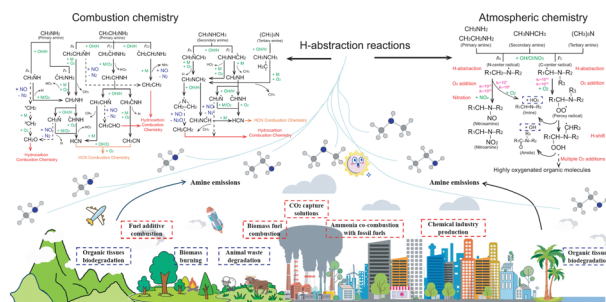
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PERSPECTIVES

20167

Insights into the role of the H-abstraction reaction kinetics of amines in understanding their degeneration fates under atmospheric and combustion conditions

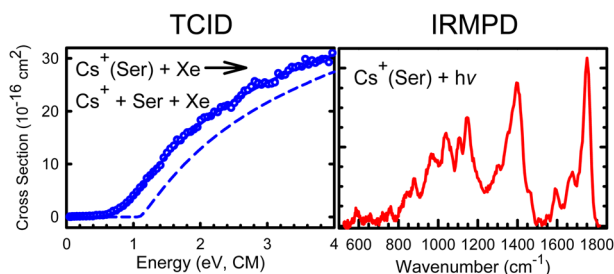
Yanlei Shang* and S. N. Luo



20216

Perspective: intrinsic interactions of metal ions with biological molecules as studied by threshold collision-induced dissociation and infrared multiple photon dissociation

P. B. Armentrout*



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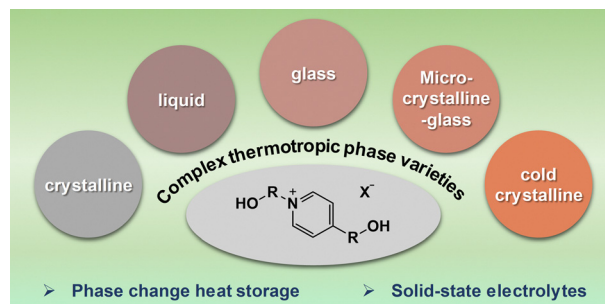


COMMUNICATIONS

20241

Complex phase behavior of dihydroxyl-functionalized ionic liquids at low temperature

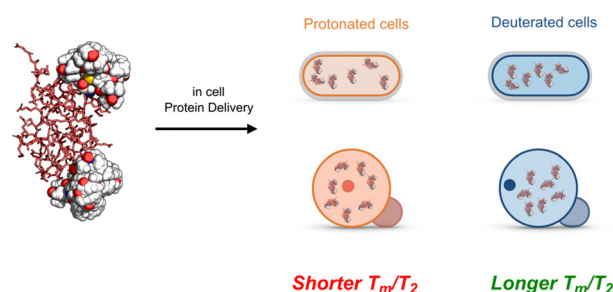
Mingjie Cui, Zeling Long, Bingxi Song, Yitong Deng, Shuwei Wang, Heng Zhang* and Guoying Zhao*



20246

A systematic study on the effect of protonation and deuteration on electron spin T_m/T_2 in a cellular context

Francesco Torricella, Valentina Vitali and Lucia Banci*

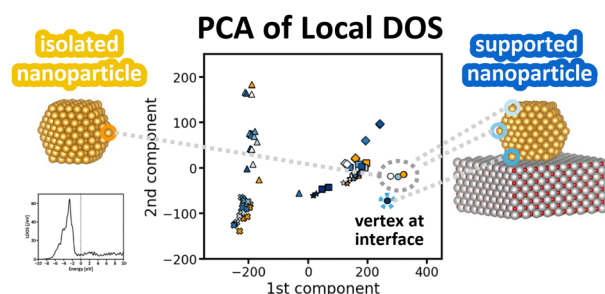


RESEARCH PAPERS

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Theoretical search for characteristic atoms in supported gold nanoparticles: a large-scale DFT study

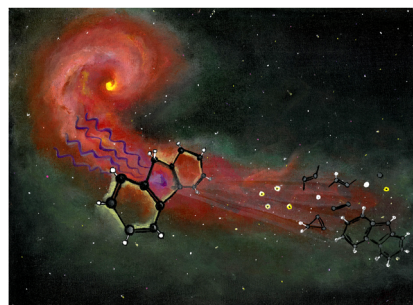
Shengzhou Li, Tsuyoshi Miyazaki and Ayako Nakata*



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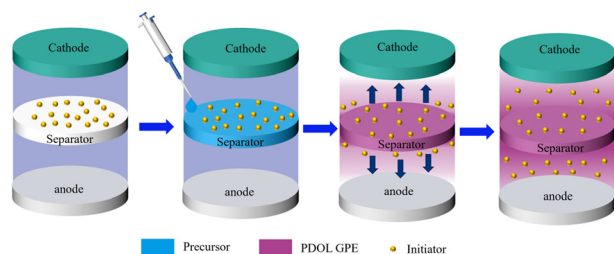
Ultrafast dynamics of fluorene initiated by highly intense laser fields

D. Garg, P. Chopra, J. W. L. Lee, D. S. Tikhonov, S. Kumar, O. Akcaalan, F. Allum, R. Boll, A. A. Butler, B. Erk, E. Gougoula, S. P. Gruet, L. He, D. Heathcote, E. Jones, M. M. Kazemi, J. Lahl, A. K. Lemmens, Z. Liu, D. Loru, S. Maclot, R. Mason, J. Merrick, E. Müller, T. Mullins, C. C. Papadopoulou, C. Passow, J. Peschel, M. Plach, D. Ramm, P. Robertson, D. Rompotis, A. Simao, A. L. Steber, A. Tajalli, A. Tul-Noor, N. Vadassery, I. S. Vinklārek, S. Techert, J. Küpper, A. M. Rijs, D. Rolles, M. Brouard, S. Bari, P. Eng-Johnsson, C. Vallance, M. Burt, B. Manschwetus and M. Schnell*



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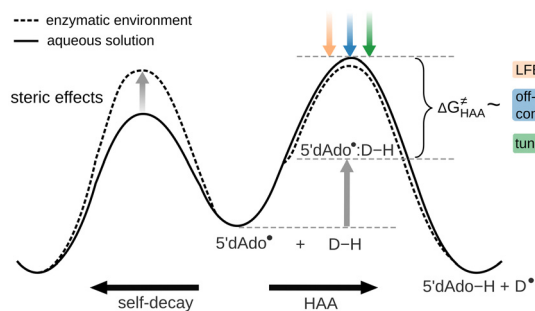
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An initiator loaded separator triggering *in situ* polymerization of a poly(1,3-dioxolane) quasi-solid electrolyte for lithium metal batteries

Hao Huang, Chaohui Wei, Qiang Zhao, Aijun Zhou and Jingze Li*

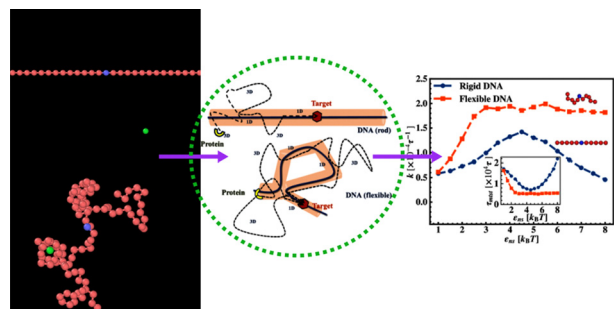
20280



Elucidation of factors shaping reactivity of 5'-deoxyadenosyl – a prominent organic radical in biology

Zuzanna Wojdyla, Mauricio Maldonado-Dominguez, Priyam Bharadwaz, Martin Culka and Martin Srnc*^{*}

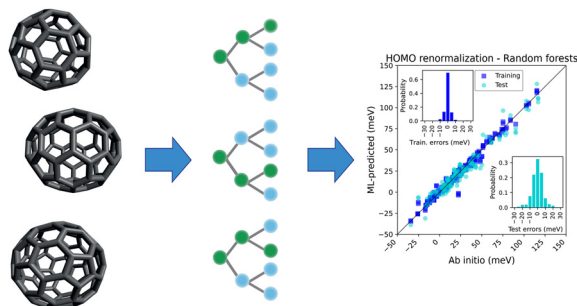
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Probing the modulation in facilitated diffusion guided by DNA-protein interactions in target search processes

Diljith Thonnekottu and Debarati Chatterjee*

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Electron-vibrational renormalization in fullerenes through *ab initio* and machine learning methods

Pablo García-Risueño,* Eva Armengol, Ángel García-Cerdaña, Juan María García-Lastra and David Carrasco-Busturia*

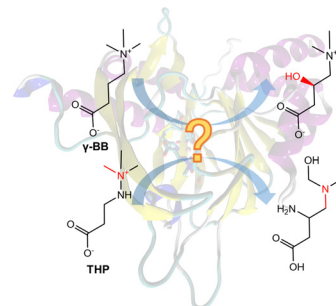


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Theoretical investigation of the reaction mechanism of THP oxidative rearrangement catalysed by BBOX

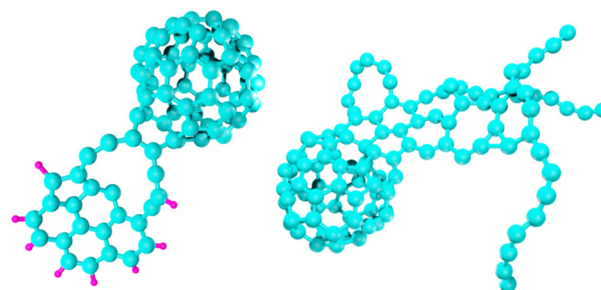
Fanqi Meng, Lu Sun, Yueying Liu, Xiang Li, Hongwei Tan,* Chang Yuan* and Xichen Li



20340

Bond breaking and making in mixed clusters of fullerene and coronene molecules induced by keV-ion impact

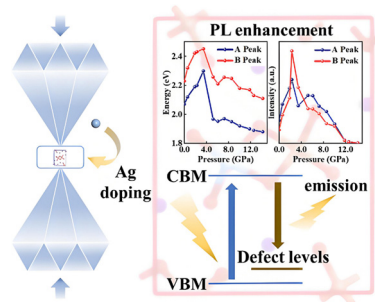
Naemi Florin, Alicja Domaracka, Patrick Rousseau, Michael Gatchell* and Henning Zettergren



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High-pressure effects on the electronic properties and photoluminescence of Ag-doped CsCu₂I₃

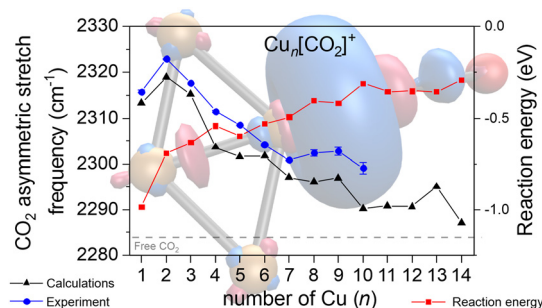
Zan Dou, Zhihua Lin, Rong Wang, Mengmeng Han, Jianxu Ding, Haoyu Wang, Xiaoguang Luo, Yingchun Cheng* and Nannan Han*



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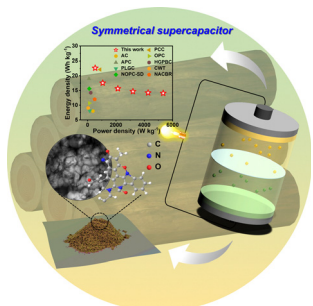
Spectroscopic investigation of size-dependent CO₂ binding on cationic copper clusters: analysis of the CO₂ asymmetric stretch

A. M. Reider, M. Szalay, J. Reichegger, J. Barabás, M. Schmidt, M. Kappe, T. Höltzl,* P. Scheier and O. V. Lushchikova*



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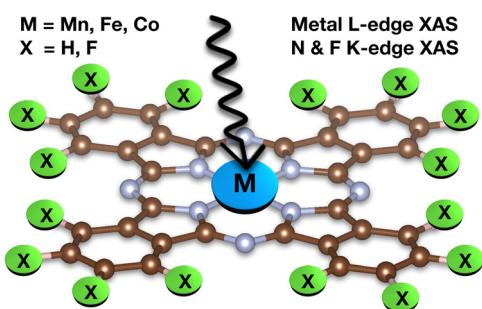
20365



Acid-modified biomass-based N-doped O-rich hierarchical porous carbon as a high-performance electrode for supercapacitors

Yuanzun Fu, Yuan Yuan, Qian Shen, Hao Xu, Zheng Ye, Li Guo, Xiaoliang Wu* and Yunhe Zhao*

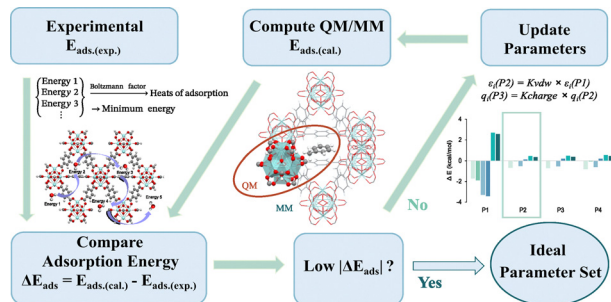
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The trials and triumphs of modelling X-ray absorption spectra of transition metal phthalocyanines

Esma Birsan Boydas and Michael Roemelt*

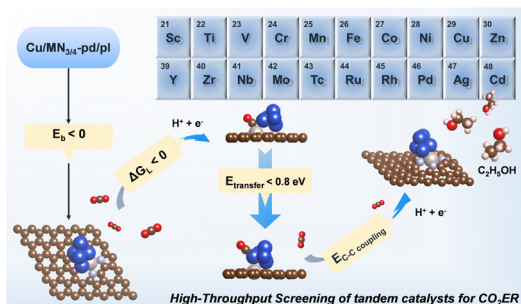
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Tailoring parameters for QM/MM simulations: accurate modeling of adsorption and catalysis in zirconium-based metal-organic frameworks

Yu-Chi Kao, Yi-Ming Wang, Jyun-Yi Yeh, Shih-Cheng Li, Kevin C.-W. Wu,* Li-Chiang Lin* and Yi-Pei Li*

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Mechanistic insights into high-throughput screening of tandem catalysts for CO₂ reduction to multi-carbon products

Yingnan Liu, Dashuai Wang,* Bin Yang, Zhongjian Li, Tao Zhang, Raul D. Rodriguez, Lecheng Lei and Yang Hou*

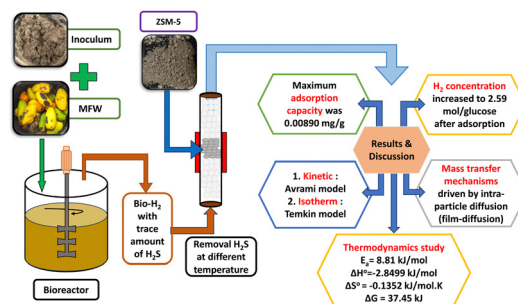


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Unravelling the kinetics, isotherms, thermodynamics, and mass transfer behaviours of Zeolite Socony Mobil - 5 in removing hydrogen sulphide resulting from a dark fermentative biohydrogen production process

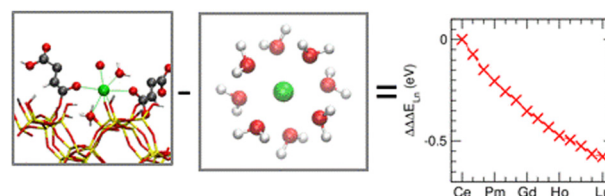
Muhammad Khairul Adha Asman, Nabilah Aminah Lutpi,* Yee-Shian Wong, Soon-An Ong, Muhammad Adli Hanif, Naimah Ibrahim, Farrah Aini Dahalan, Wirach Taweepreda and Raja Nazrul Hakim Raja Nazri



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Modeling separation of lanthanides via heterogeneous ligand binding

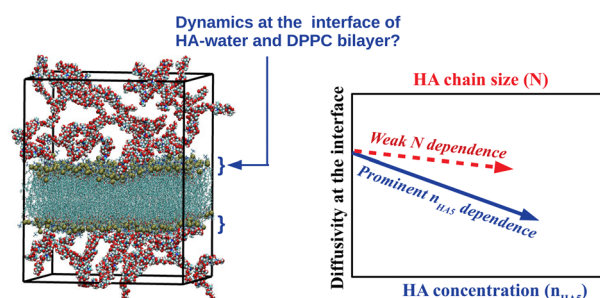
Kevin Leung* and Anastasia G. Ilgen



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Dynamics of an aqueous suspension of short hyaluronic acid chains near a DPPC bilayer

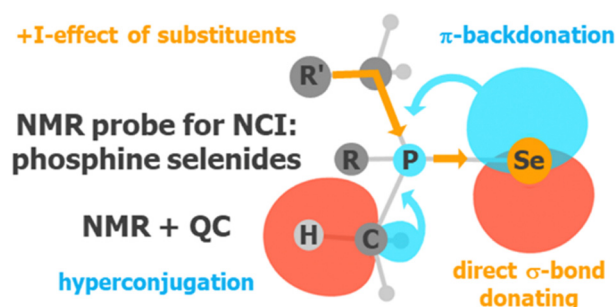
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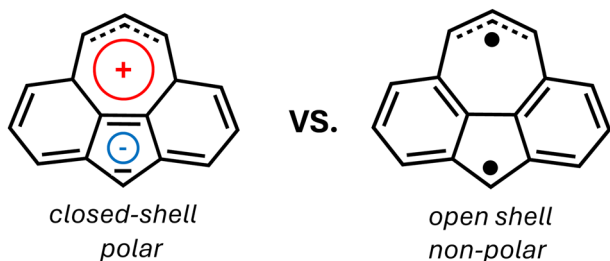
Unveiling the electronic structure peculiarities of phosphine selenides as NMR probes for non-covalent interactions: an experimental and theoretical study

Danil V. Krutin, Anton S. Zakharov, Elena Yu. Tupikina and Valeriya V. Mulloyarova*



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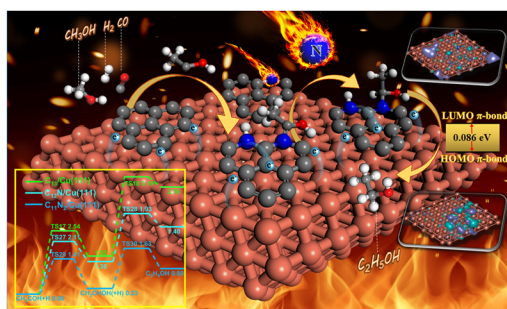
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Cyclohepta[def]fluorene as a bistable molecule: first principles studies on its electronic structure and the effects of benzo-extension, substitution and solvation

Robert Toews* and Andreas Köhn

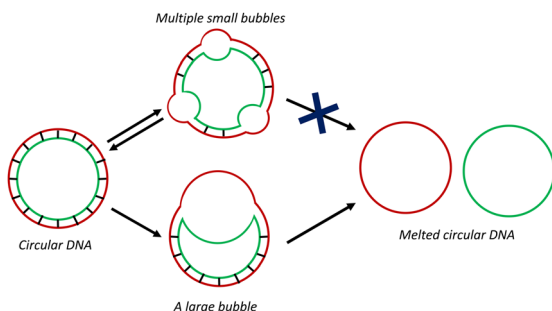
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On the nature of Cu-carbon interaction through N-modification for enhanced ethanol synthesis from syngas and methanol

Mingxue Yang, Bing Bai, Hui Bai,* Zhongzeng Wei, Haojie Cao, Zhijun Zuo, Zhihua Gao, Vladimir A. Vinokurov, Jianping Zuo, Qiang Wang and Wei Huang*

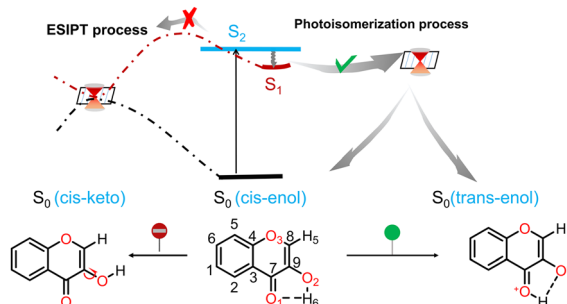
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Large bubble drives circular DNA melting

Souradeep Sengupta, Somendra M. Bhattacharjee and Garima Mishra*

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Excited-state dynamics of 3-hydroxychromone in gas phase

Li Zhao,* Xuehui Geng, Jiangyue Wang, Yuxuan Liu, Wenhui Yan, Zhijie Xu and Junsheng Chen*

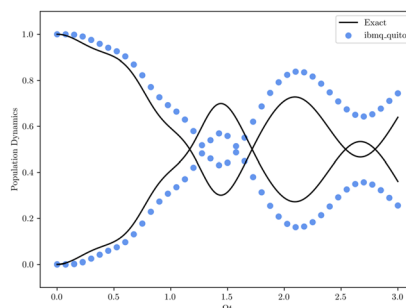


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An ensemble variational quantum algorithm for non-Markovian quantum dynamics

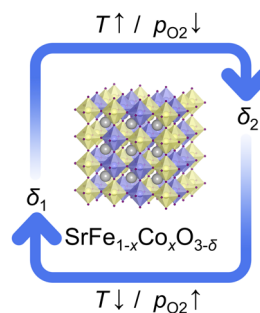
Peter L. Walters, Joachim Tsakanikas and Fei Wang*



20511

An investigation of the structural and electronic origins of enhanced chemical looping air separation performance of B-site substituted $\text{SrFe}_{1-x}\text{Co}_x\text{O}_{3-\delta}$ perovskites

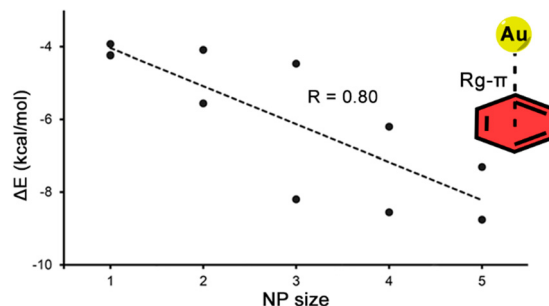
Qianwenhao Fan, Haiyan Li, Syed Saqline, Felix Donat, Mingwu Tan, Longgang Tao, Christoph R. Müller, Zhichuan J. Xu and Wen Liu*



20522

On the influence of metal nanoparticle and π -system sizes in the stability of noncovalent adducts: a theoretical study

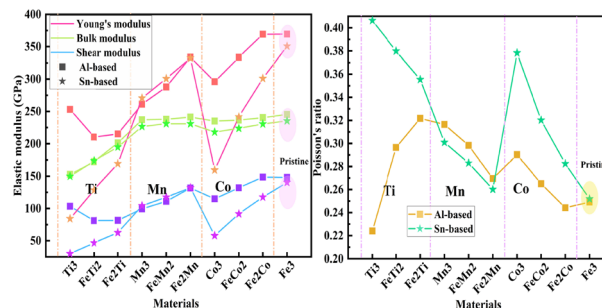
Sergi Burguera, María de las Nieves Piña and Antonio Bauzá*



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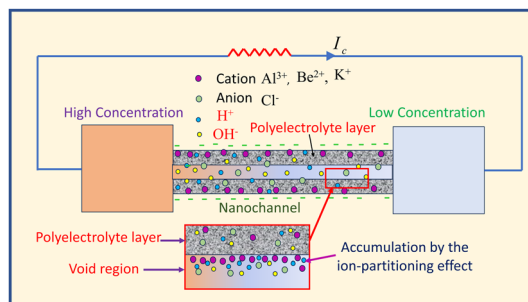
First-principles investigations of Fe-based A_3BX ceramics with high stiffness and damage tolerance

Tianyu Tang and Yanlin Tang*



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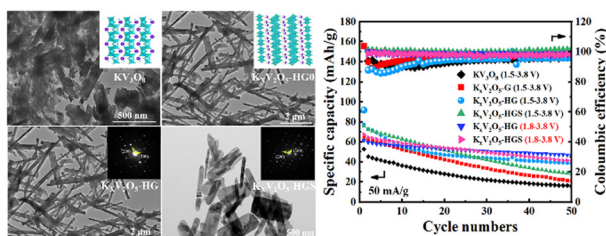
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Maximizing blue energy: the role of ion partitioning in nanochannel systems

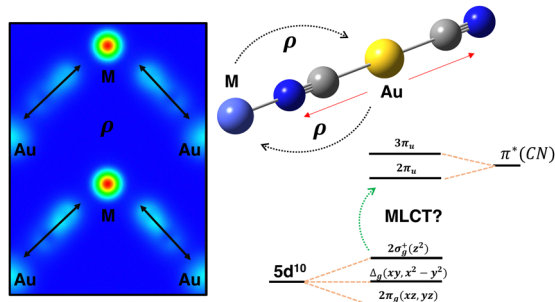
Sumit Kumar Mehta, Debarthy Deb, Adhiraj Nandy, Amy Q. Shen and Pranab Kumar Mondal*

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Crystallization and electrochemical properties of $K_xV_2O_5$ nano-ribbons obtained via a solvothermal process as a promising cathode for PIBs

Zhiwei Ding, Junyuan Huang, Yuan Xie, Xiping Wang, Rong Jiang, Jia Wen, Xinyu Li, Wenli Zhang, Yang Ren, Zhu Liu, Xu Chen and Xiaowei Zhou*

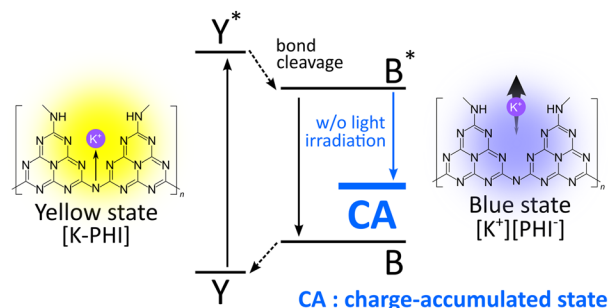
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A first principles study of the electronic structure and optical response of heterobimetallic M-dicyanoaurate-based coordination polymers (M = Mn, Co, Ni, Zn and Cd)

R. Mojica,* M. C. Vázquez, A. E. Torres, Y. Avila, R. Borja-Urby, J. Rodriguez-Hernández and E. Reguera*

20585



Mechanism of charge accumulation in potassium poly(heptazine imide)

Goichiro Seo,* Ryoma Hayakawa, Yutaka Wakayama, Ryosuke Ohnuki, Shinya Yoshioka and Kaname Kanai

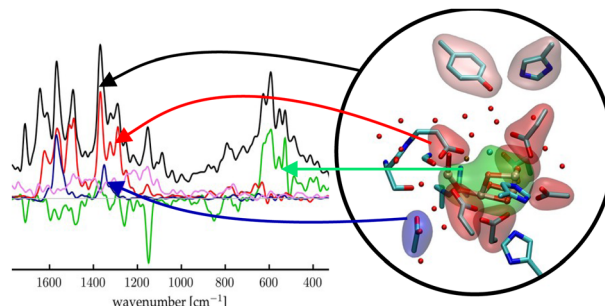


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Unravelling Mn_4Ca cluster vibrations in the S_1 , S_2 and S_3 states of the Kok–Joliot cycle of photosystem II

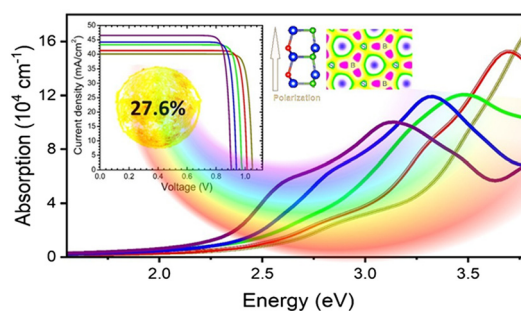
Matteo Capone,* Gianluca Parisse, Daniele Narzi and Leonardo Guidoni*



20610

A new highly stable multifunctional two-dimensional Si_2BN monolayer quantum material with a direct bandgap predicted by density functional theory

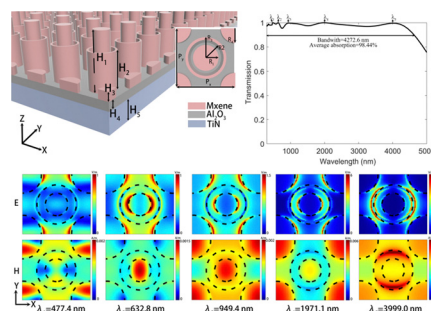
Bezzerga Djamel, Naouel Chelil, Sahnoun Mohammed, Sergey Gusarov, Gap Soo Chang and Mosayeb Naseri*



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A wide angle broadband solar absorber with a horizontal multi-cylinder structure based on an MXene material

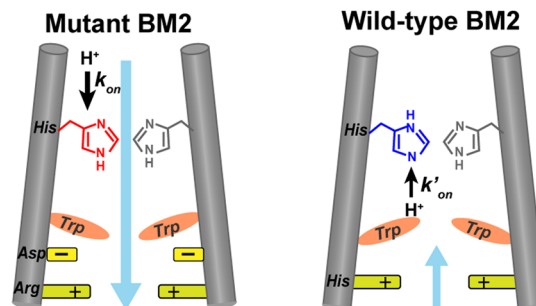
Yuchang Li, Fang Chen,* Wenxing Yang* and Shaolin Ke



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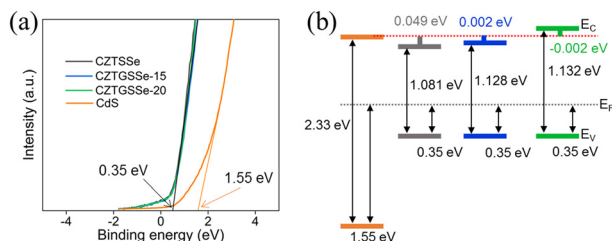
Structure and dynamics of the proton-selective histidine and the gating tryptophan in an inward rectifying hybrid influenza B and A virus M2 proton channel

Yanina Pankratova, Matthew J. McKay, Chunlong Ma, Haozhou Tan, Jun Wang and Mei Hong*



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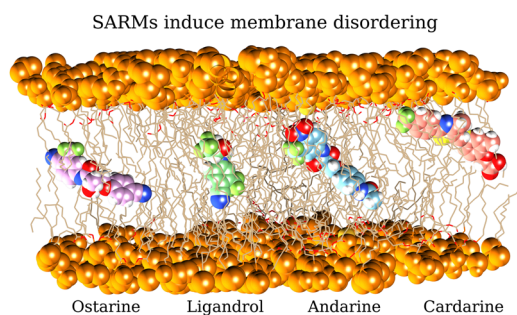
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Improving the performance of kesterite solar cells by solution germanium alloying

Sitong Xiang, Yize Li, Chunxu Xiang, Hongkun Liu, Yuanyuan Zheng, Shaoying Wang,* Weibo Yan* and Hao Xin*

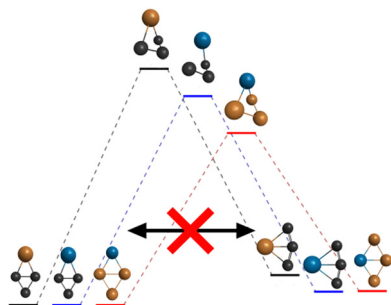
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The disordering effect of SARMs on a biomembrane model

Alma Jessica Díaz-Salazar, Arián Espinosa-Roa,* Enrique Saldivar-Guerra* and Rosendo Pérez-Isidoro*

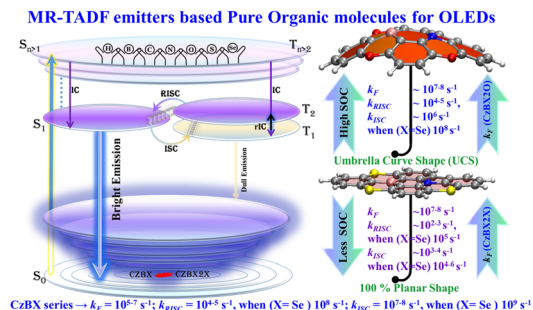
20663



An investigation into transition states of cyclic tetra-atomic silicon and germanium interstellar dust compounds: $\text{Si}_x\text{C}_{4-x}$, $\text{Ge}_x\text{C}_{4-x}$, and $\text{Ge}_x\text{Si}_{4-x}$ ($x \in \{1,2,3\}$)

A. Mackenzie Flowers, Alex Brown* and Mariusz Klobukowski*

20672



Unveiling the photophysical and excited state properties of multi-resonant OLED emitters using combined DFT and CCSD method

Pandiyan Sivasakthi and Pralok K. Samanta*

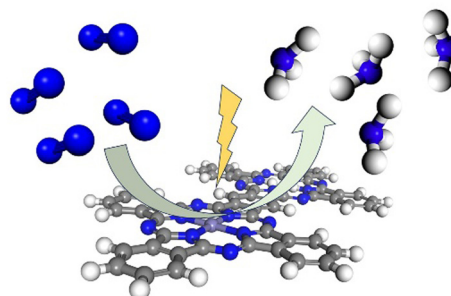


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20684

Modulating the electronic structure of ion phthalocyanine-based molecular catalysts for electrocatalytic nitrogen reduction: a DFT study

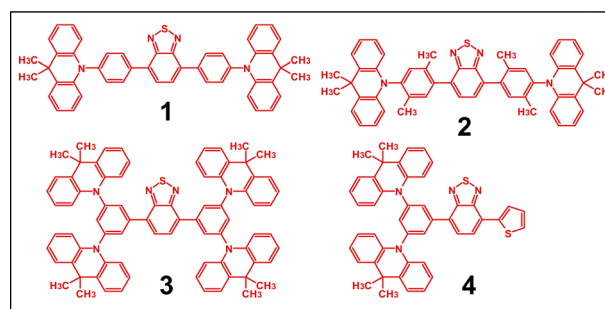
Ze-Yuan Wu, Jiaju Fu and Jin-Song Hu*



20690

Photophysical and redox properties of new donor–acceptor–donor (DAD) compounds containing benzothiadiazole (A) and dimethyldihydroacridine (D) units: a combined experimental and theoretical study

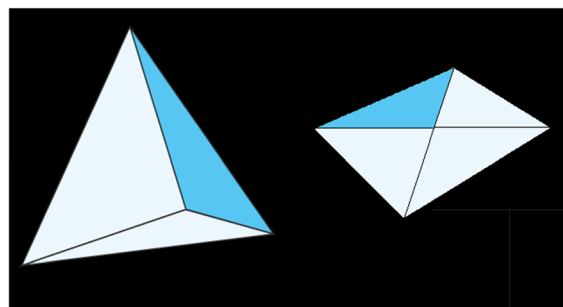
Emilia Polesiak, Malgorzata Makowska-Janusik, Jakub Drapala, Malgorzata Zagorska, Marzena Banasiewicz, Boleslaw Kozankiewicz, Irena Kulszewicz-Bajer* and Adam Pron*



20701

On the variation of cluster core characteristics by an endohedral atom. Shape variation in 8-ce $[EAu_4(PPh_3)_4]^{2+}$ (E = N, P, As, Sb) clusters

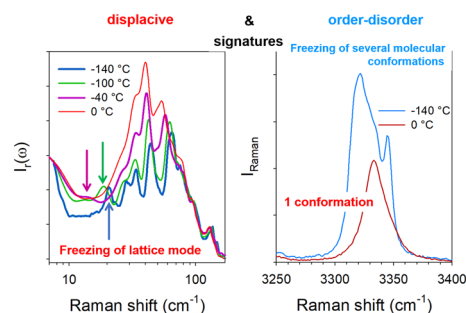
Raul Guajardo-Maturana, Desmond MacLeod Carey, Peter L. Rodriguez-Kessler and Alvaro Muñoz-Castro*



20709

Description of an original molecular ordering process into a disordered crystalline form: the atypical low-temperature transformation of the disordered form III of linezolid

Mehrnaz Khalaji, Marta Katarzyna Dudek, Laurent Paccou, Florence Danède, Yannick Guinet and Alain Hédoux*



CORRECTION

20717

Correction: Simple, accurate, adjustable-parameter-free prediction of NMR shifts for molecules in solution

Emlyn M. Hoyt, Lachlan O. Smith and Deborah L. Crittenden*

