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ISSN 1463-9076 CODEN PPCPFQ 26(42) 26631–27226 (2024)



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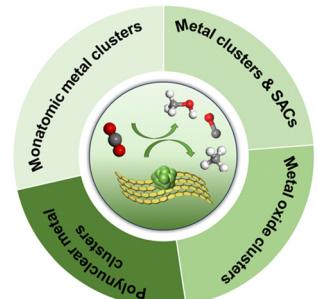
See Hao Su, Xiang Sheng et al., pp. 26677–26692.
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REVIEW

26647

Applications of metal nanoclusters supported on the two-dimensional material graphene in electrocatalytic carbon dioxide reduction

Shanlin Chen, Haiyan Zhu,* Tingting Li, Ping Liu, Chou Wu, Shaobo Jia, Yawei Li* and Bingbing Suo

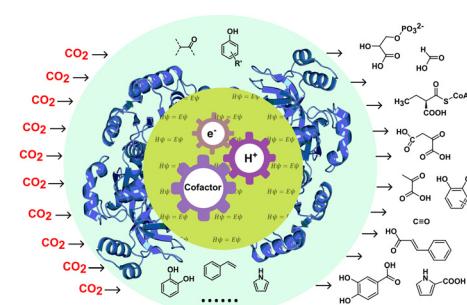


PERSPECTIVES

26677

Quantum chemical studies of the reaction mechanisms of enzymatic CO_2 conversion

Baoyan Liu, Beibei Lin, Hao Su* and Xiang Sheng*



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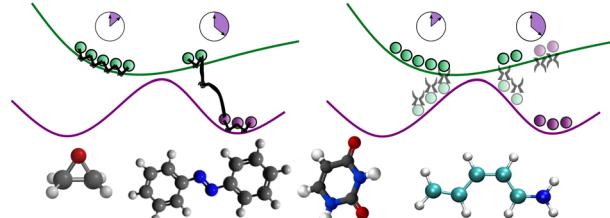
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Simulations of photoinduced processes with the exact factorization: state of the art and perspectives

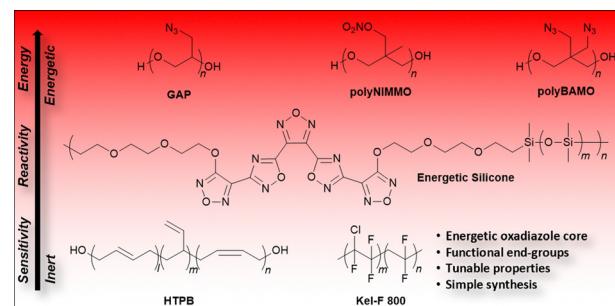
Lea Maria Ibele, Eduarda Sangiogo Gil,
Evaristo Villaseco Arribas and Federica Agostini*EXACT FACTORIZATION
Coupled Trajectories Auxiliary Trajectories

COMMUNICATIONS

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Energetic silicones: synthesis and characterization of pentaoxadiazole-PDMS copolymers

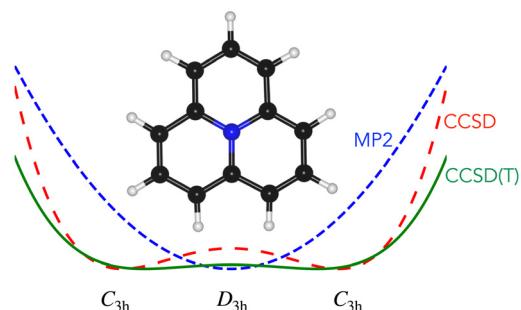
Trevor A. Shear, Anthony J. Varni, Mao-Xi Zhang* and H. Paul Martinez*



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Influence of pseudo-Jahn–Teller activity on the singlet–triplet gap of azaphenalenes

Atreyee Majumdar, Komal Jindal, Surajit Das and Raghunathan Ramakrishnan*

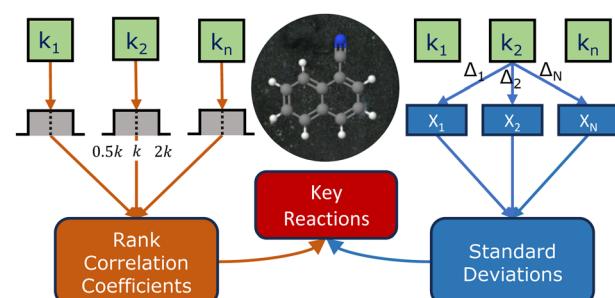


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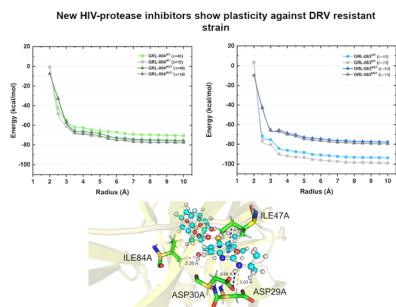
Sensitivity analysis of aromatic chemistry to gas-phase kinetics in a dark molecular cloud model

Alex N. Byrne,* Ci Xue, Troy Van Voorhis and Brett A. McGuire*



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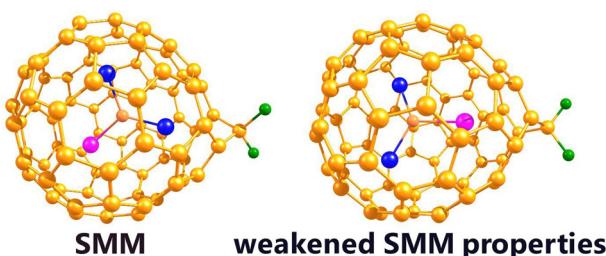
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Quantum mechanical analysis of newly synthesized HIV-1 protease inhibitors: evaluation of wild-type and resistant strain binding interactions

Gabriel Vinícius Rolim Silva, Klaus Augustus Ramos Reiniger, Gabriela de Lima Menezes, Katyanna Sales Bezerra, Douglas Soares Galvão, Marielena Vogel Saivish, Roosevelt Alves da Silva, Shopnil Akash, Jehad Zuhair Tayyeb, Jonas Ivan Nobre Oliveira and Umberto Laino Fulco*

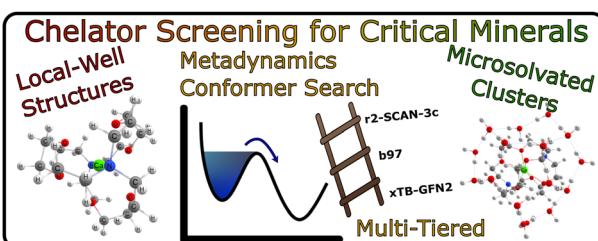
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Effect of exohedral functionalization on the magnetic properties in the dysprosium-containing endohedral fullerene $\text{DySc}_2\text{N}@C_{80}(\text{CF}_2)$

Viktor E. Khinevich, Svetlana M. Sudarkova and Ilya N. Ioffe*

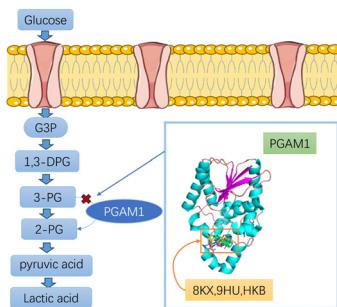
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Cryptate binding energies towards high throughput chelator design: metadynamics ensembles with cluster–continuum solvation

Sean M. Nations, Lauren C. Burrows, Scott E. Crawford and Wissam A. Saidi*

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Accelerated molecular dynamics study of the interaction mechanism between small molecule inhibitors and phosphoglycerate mutase 1

Yanqi Sun, Chaoyue Jia, Shaolong Zhang, Qinggang Zhang, Jianzhong Chen* and Xinguo Liu*

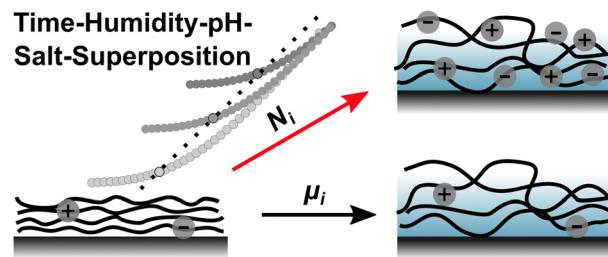


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Time-pH and time-humidity scaling of ionic conductivity spectra of polyelectrolyte multilayers

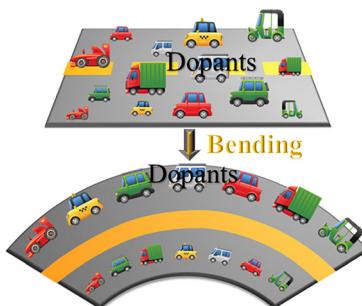
Jannis Schlicke, Cornelia Cramer* and Monika Schönhoff*



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Bending-induced enhanced spatial separation of dopants and long-lived conventional nanoribbon p–n junctions

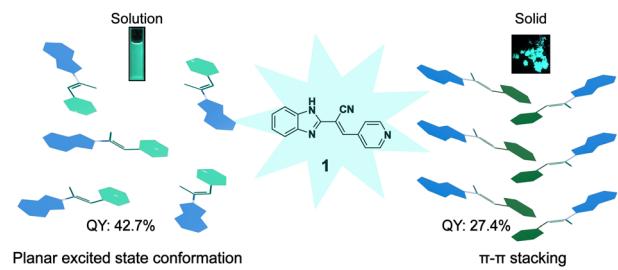
Xu Liu, Yu-Run Yang, Jing Wang, Rui-Ping Xu, Zhao Liu* and Ying Liu



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Solution and solid-state fluorescence emission from cyanostyrene molecules with multiple nitrogen atoms

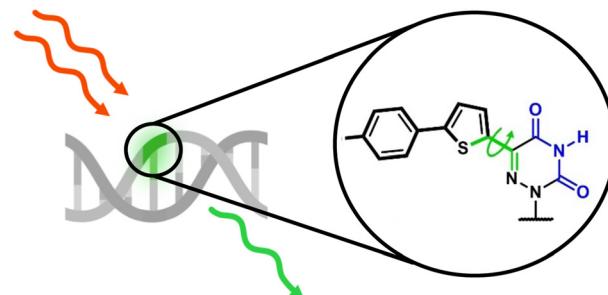
Yang Chen, Smruti Ranjan Sahoo, Glib V. Baryshnikov,* Lei Gao,* Zhijia Zhu* and Hongwei Wu*



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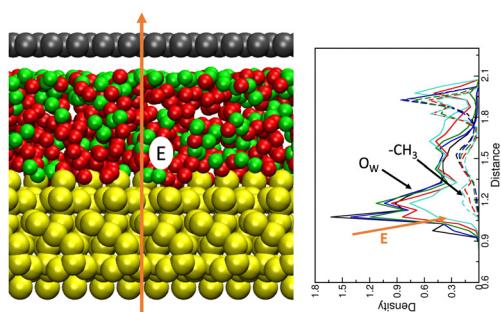
Ultrasensitive detection of a responsive fluorescent thymidine analogue in DNA via pulse-shaped two-photon excitation

Alexandra E. Bailie, Henry G. Sansom, Rachel S. Fisher, Ryo Watabe, Yitzhak Tor, Anita C. Jones* and Steven W. Magennis*



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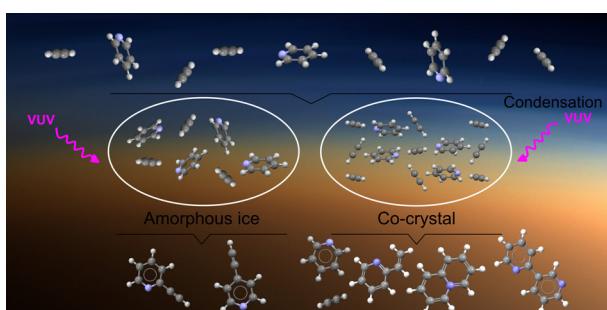
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Electric-field-induced structure and dynamics of an ethanol–water mixture in hydrophobic–hydrophilic nanochannels

Abir Ghosh,* Sunandini Swain and Atanu K. Metya*

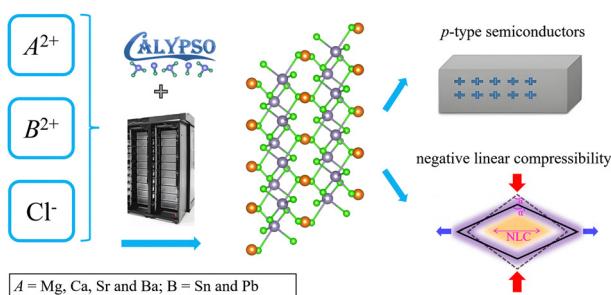
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Vacuum-ultraviolet irradiation of pyridine:acetylene ices relevant to Titan astrochemistry

Larissa Lopes Cavalcante, Ellen C. Czaplinski, Helen E. Maynard-Casely, Morgan L. Cable, Naila Chaouche-Mechidal, Robert Hodyss and Courtney Ennis*

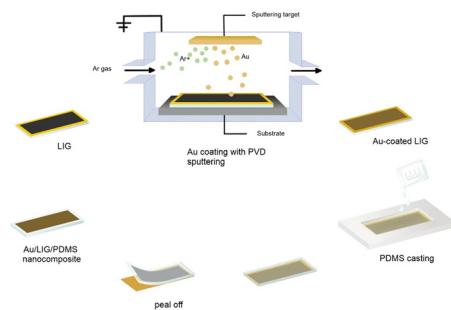
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Prediction of ternary alkaline-earth metal Sn(II) and Pb(II) chlorides with potential applications as p-type transparent conductors

Li Wang, Tingting Lin, Jia Wang, Chao Fang, Yuwei Li* and Yuancun Qiao*

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Wearable gold decorated direct laser writing graphene for ultra-minor strains

Elnaz Khakpour and Sadegh Sadeghzadeh*

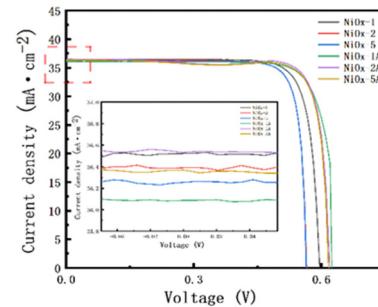


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Effects of adjusting nickel pulse count on NiO_x films prepared by atomic layer deposition

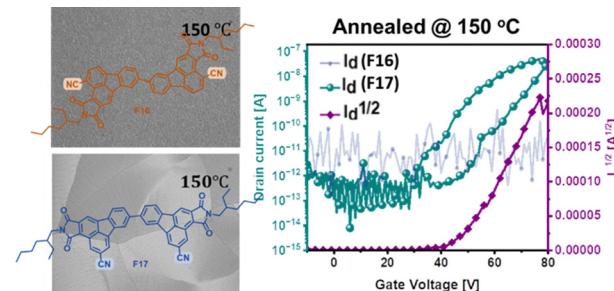
Xuanfei Kuang, Zongtao Liu, Yang Hong, Yongjuan Chen, Yao Xiao and Zongcun Liang*



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Fluoranthene imide dimers with strong isomeric effects on the charge transport properties

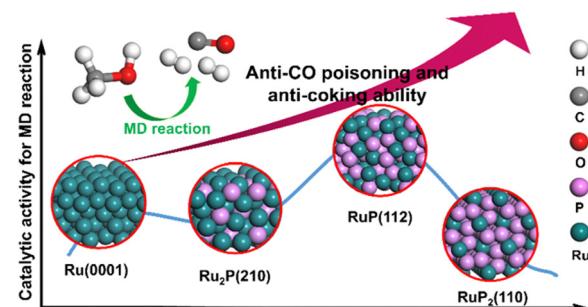
Ting-Yu Wang, Huangcheng Liu, Miao Liu, Yen-Han Shih, Xinyu Yu, Zhong'an Li* and Chu-Chen Chueh*



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DFT study on the mechanism of methanol dehydrogenation over Ru_xP_y surfaces

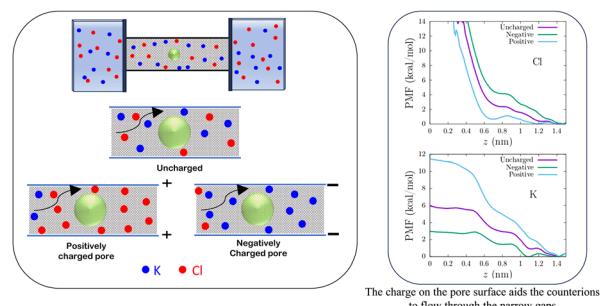
Hao Lu, Yuan Zhong, Yao Jie, Pan Yin, Tian-Yao Shen, Jing-Yi Guo, Min Pu and Hong Yan*



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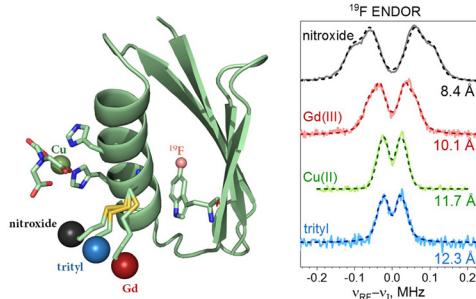
Ionic flow through partially blocked nanopores

Sipra Mohapatra, Hema Teherpuria, Santosh Mogurampelly, Matthew Downton and Sridhar Kumar Kannam*



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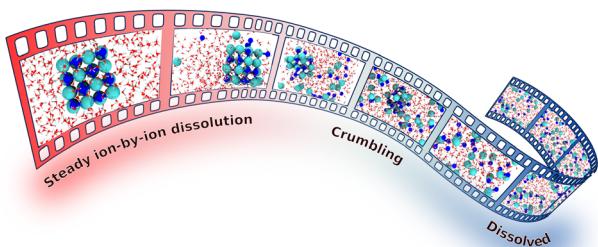
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Spin labels for ^{19}F ENDOR distance determination: resolution, sensitivity and distance predictability

Alexey Bogdanov,* Longfei Gao, Arina Dalaloyan, Wenkai Zhu, Manas Seal, Xun-Cheng Su, Veronica Frydman, Yangping Liu, Angela M. Gronenborn and Daniella Goldfarb*

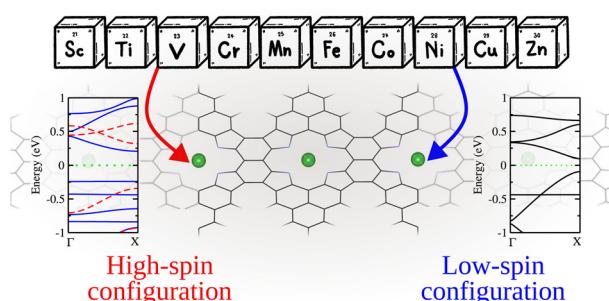
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Crumbling crystals: on the dissolution mechanism of NaCl in water

Niamh O'Neill, Christoph Schran,* Stephen J. Cox and Angelos Michaelides*

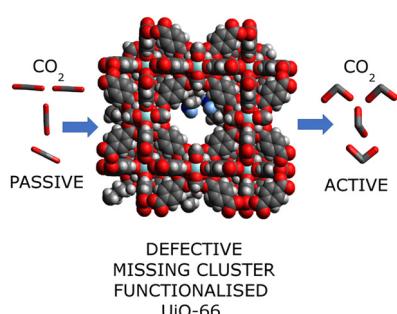
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Electronic and magnetic properties of porphyrin nanoribbons with chelated metals

Thainá Araújo Oliveira,* Paloma Vieira Silva, Fabrício Morais de Vasconcelos, Vincent Meunier and Eduardo Costa Girão*

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Computationally aided design of defect-appended aliphatic amines for CO_2 activation within UiO-66

Gerard Pareras, Albert Rimola, Marco Taddei* and Davide Tiana*

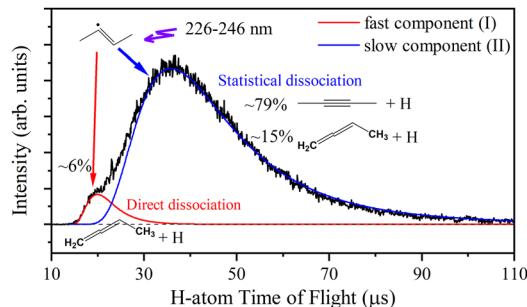


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Ultraviolet photochemistry of the 2-buten-2-yl radical

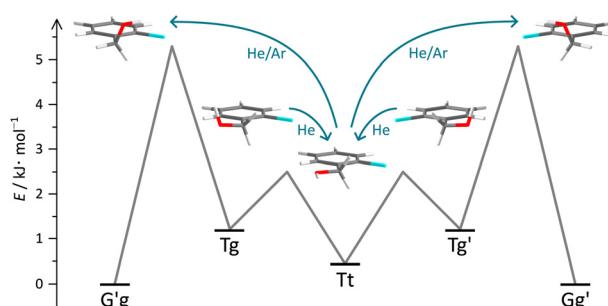
Michael Lucas, Yuan Qin, Lei Yang, Ge Sun and Jingsong Zhang*



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Controlling achiral and chiral conformations of benzyl alcohol by *ortho*-halogenation, collisional relaxation and dimerisation

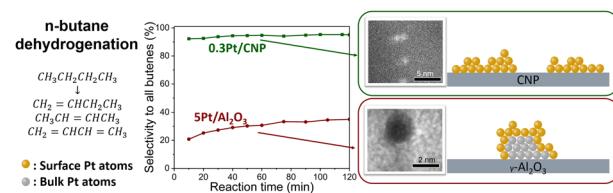
Elisabeth Sennert and Martin A. Suhm*



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Unprecedented selectivity behavior in the direct dehydrogenation of *n*-butane to *n*-butenes with similar active Pt nanoparticle size: unveiling structural and electronic characteristics of supported monometallic catalysts

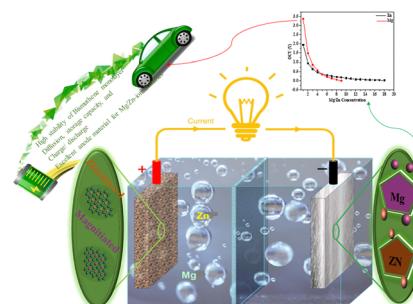
Gustavo Enrique Ramos Montero,* Adriana Daniela Ballarini, María Julia Yañez, Sergio Rubén de Miguel, Sonia Alejandra Bocanegra and Patricia Daniela Zgolcic



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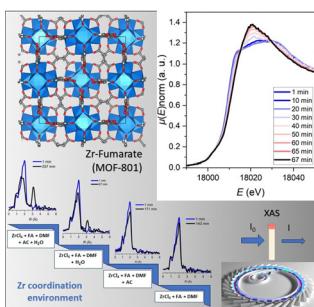
Bismuthene as a novel anode material of magnesium/zinc ion batteries with high capacity and stability: a DFT calculation

Muhammad Isa Khan,* Mahnaz Khurshid, Saleh S. Alarfaji and Abdul Majid



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Exploring cluster formation in Zr-MOF synthesis *in situ* using X-ray absorption spectroscopy

Olena Zavorotynska,* Anna Cecilie Åstrand, Pascal D. C. Dietzel and Sachin M. Chavan*

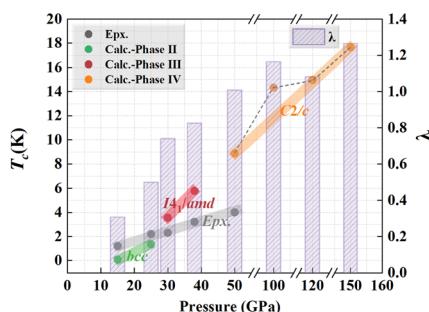
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Helium cluster ions: coherent charge sharing and the general trimerization trend

Laura Van Dorn and Andrei Sanov*

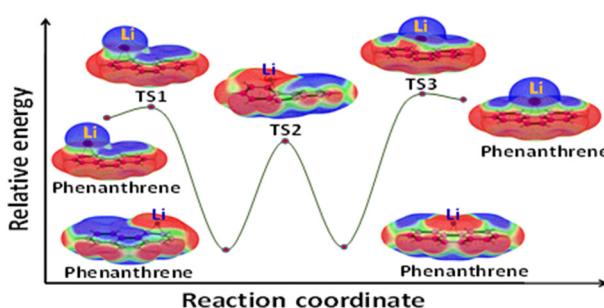
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Compressed Sr superconducting transition temperature up to 17.65 K

Ya-Le Tao, Qi-Jun Liu,* Dai-He Fan, Fu-Sheng Liu and Zheng-Tang Liu

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From loose to tight: unveiling bond stretch isomerism in π -complexes of Li, Na and K

Pilankatta K. Ramya, Ayush Shivhare, Milind M. Deshmukh and Cherumuttathu H. Suresh*

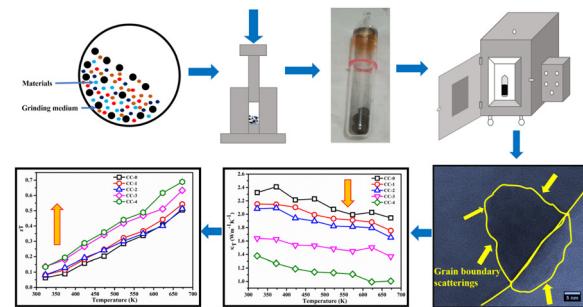


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Synergistic optimization of thermoelectric properties in $\text{Cu}_2\text{NiSnSe}_4$ composited with CuO nanoparticles

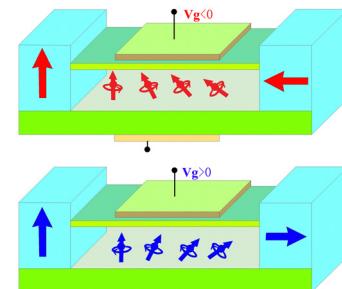
J. Mani, S. Radha, J. Kiruthika, Ajith Kumar Lakshmanan, M. Arivanandhan and G. Anbalagan*



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Gated spin manipulation in a bipolar Rashba semiconductor: a Janus TeSSe monolayer

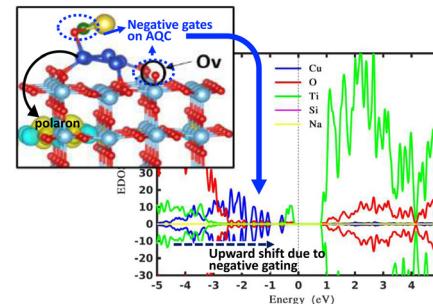
Shao-Bo Chen,* Wan-Jun Yan and Yee Sin Ang*



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Theoretical investigation of Cu_5 /silicates deposited on rutile TiO_2 as a photocatalyst

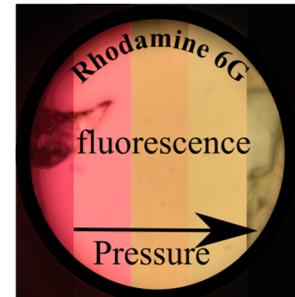
Fatimah Alhawiti, Qingqing Wu,* David Buceta, Songjun Hou, M. Arturo López-Quintela and Colin Lambert*



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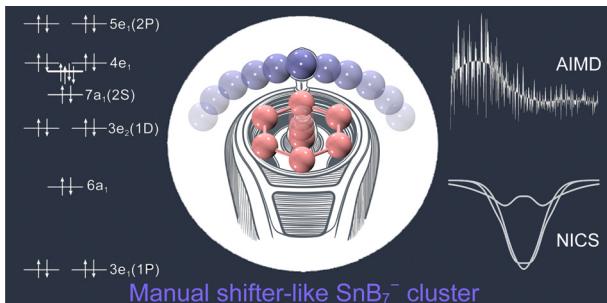
Fluorescence and absorption of rhodamine 6G solutions as pressure standards for a diamond-anvil cell

Ida Moszczyńska, Anna Golczak, Marek Sikorski and Andrzej Katrusiak*



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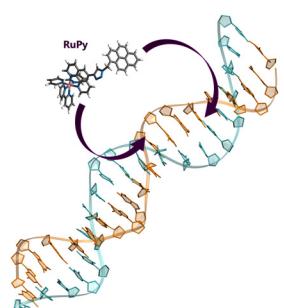
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Discovering SnB_7^- : a half-sandwich structure with double aromaticity and pathways to molecular machines

Yong-Hang Zhang, Huai-Qian Wang,* Hui-Fang Li,* Jia-Ming Zhang, Hao Zheng, Kai-Le Jiang, Bo Zhang and Wen-Hai Wu

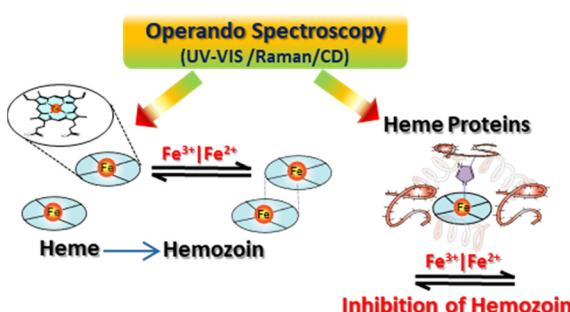
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Binding modes of a flexible ruthenium polypyridyl complex to DNA

Meritxell Malagarriga and Leticia González*

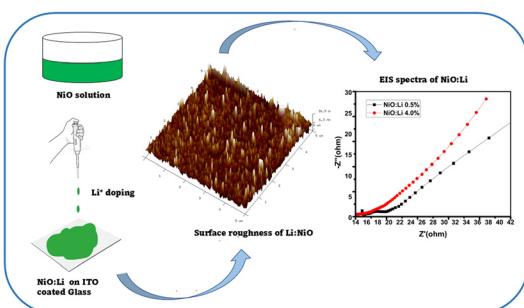
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Operando spectroscopy investigations of the redox reactions in heme and heme-proteins

Subhankar Mandal, Dipen Biswakarma and Aninda J. Bhattacharyya*

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Enhanced electrochemical performance of NiO surfaces via selective Li^+ doping

Tithi Sen,* Amrita Biswas,* Udayabhanu Gopalakrishnan Nair, Rajalingam Thangavel and Tapan Kumar Rout

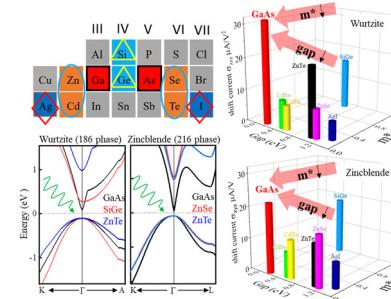


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The shift current photovoltaic effect response in wurtzite and zinc blende semiconductors via first-principles calculations

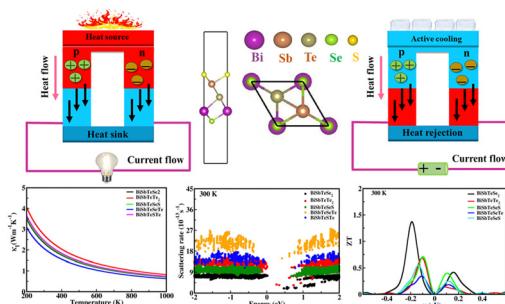
Yu Qiu, Yong Sun, Hui-Xue Shen, Hui-Xia Fu,*
Man-Yi Duan and Cai Cheng*



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Two-dimensional BiSbTeX_2 ($X = \text{S, Se, Te}$) and their Janus monolayers as efficient thermoelectric materials

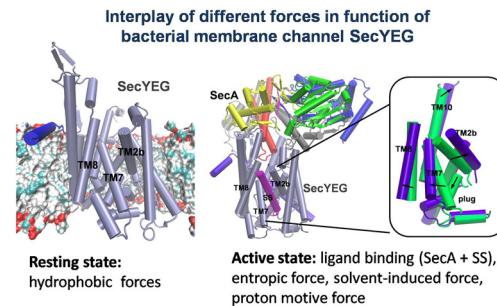
KM Sujata, Poonam Chauhan, Nidhi Verma,
Rekha Garg Solanki* and Ashok Kumar*



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Physical mechanisms of the Sec machinery operation

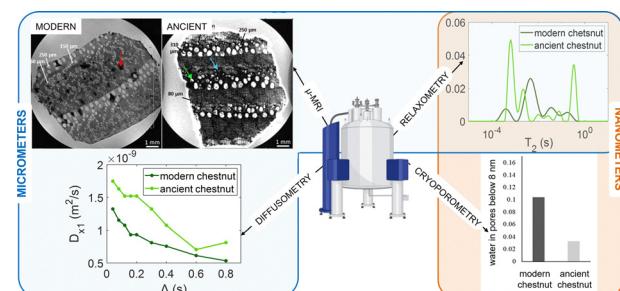
Ekaterina Sobakinskaya and Frank Müh*



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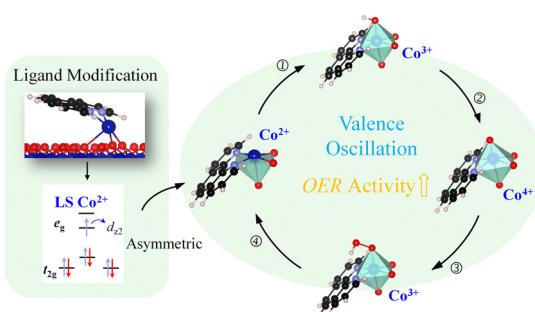
Comprehensive characterization of waterlogged archaeological wood by NMR relaxometry, diffusometry, micro-imaging and cryoporometry

Valeria Stagno,* Otto Mankinen, Sarah Mailhot,
Ville-Veikko Telkki and Silvia Capuani



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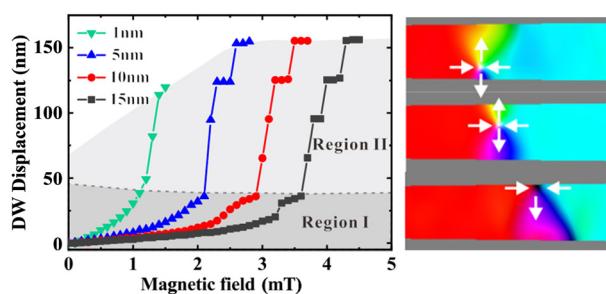
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Asymmetric electron occupation of transition metals for the oxygen evolution reaction *via* a ligand–metal synergistic strategy

Pai Wang, Kunyu Li, Tongwei Wu, Wei Ji and Yanning Zhang*

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Magnetic-field-controlled positioning of magnetic domain wall in tie-shaped asymmetric nanowire and its application for magnetic field detection

Xiaoxue Yang, Xue-Feng Zhang, Changfeng Li and Huiting Li*