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See Hui-Ting Bian, Hui-Ling Jiang, Kai-Yuan Li *et al.*, pp. 16311–16325. Image reproduced by permission of Hui-Ting Bian and Yang Wang from *Phys. Chem. Chem. Phys.*, 2025, 27, 16311.



Inside cover

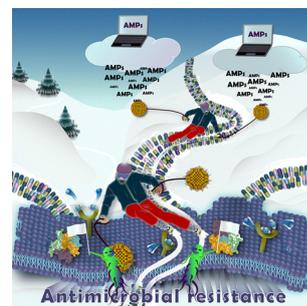
See Miroslava Nedyalkova *et al.*, pp. 16284–16294. Image reproduced by permission of Miroslava Nedyalkova from *Phys. Chem. Chem. Phys.*, 2025, 27, 16284.

PERSPECTIVE

16284

Harnessing antimicrobial peptide-functionalized nanoparticles: a perspective on experimental and computational strategies to combat antibiotic resistance

Miroslava Nedyalkova,* Diana Potes Vecini, Andrew S. Paluch and Marco Lattuada

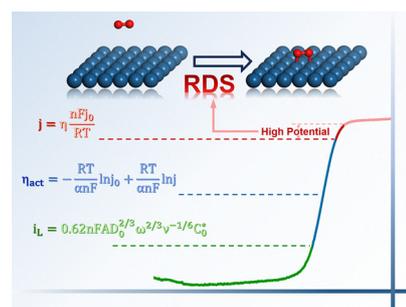


COMMUNICATIONS

16295

Confirmation of the rate-determining step for ORR in the high potential region: adsorption process of oxygen molecules on the catalyst surface

Jiayi Zeng, Jiyuan Lu, LiLi Zhang, Jijia Yang, Shengwei Yu* and Haibo Jiang*



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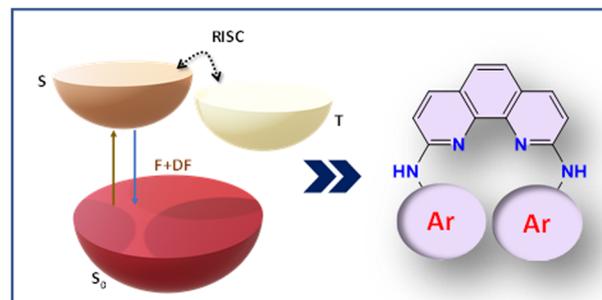
Fundamental questions
Elemental answers

COMMUNICATIONS

16301

Thermally activated delayed fluorescence in aminoacene-linked phenanthroline

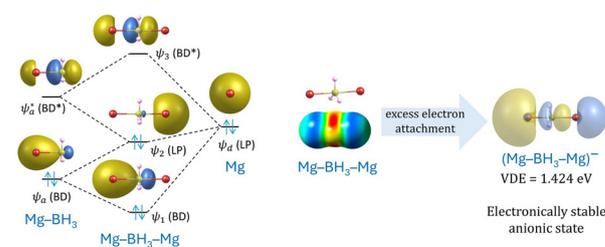
P. E. Swathi Krishna, Hanock Baiju and Mahesh Hariharan*



16306

 s^2 lone pair-driven formation of a 3-center 4-electron (3c-4e) Mg–B–Mg dative bond in neutral $\text{Mg}(\text{BH}_3)\text{Mg}$

Iwona Anusiewicz, Sylwia Freza and Piotr Skurski*

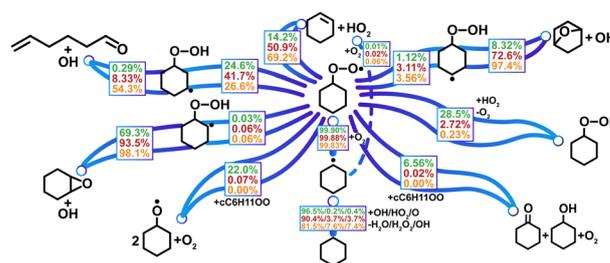
The construction of σ natural bond orbitals (donor-acceptor interaction diagram)

RESEARCH PAPERS

16311

Impact of conformational structures on low-temperature oxidation chemistry for cyclohexyl radicals: a theoretical and kinetic modeling study on first oxygen addition

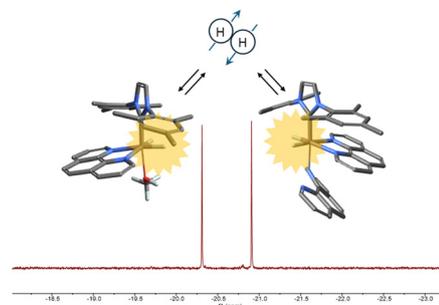
Hui-Ting Bian, Yang Wang, Shi-Hao Feng, Long Zhao, Wen-Chao Lu, Hui-Ling Jiang* and Kai-Yuan Li*



16326

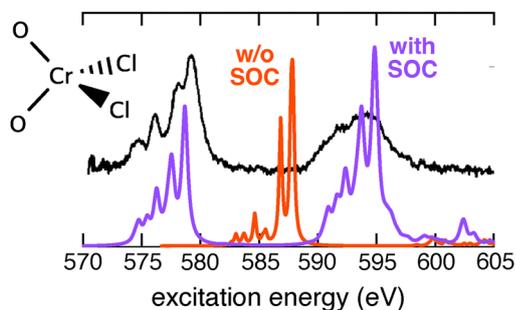
Predicting the NMR chemical shifts of hydrides in SABRE-active Ir complexes by relativistic DFT

Beatrice Bernadette Mascitti, Giordano Zanoni, Federico de Biasi, Federico Rastrelli* and Giacomo Saielli*



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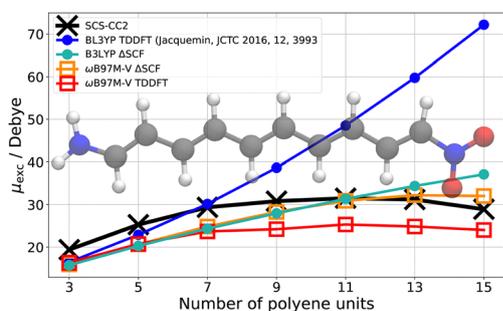
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Computing L- and M-edge spectra using the DFT/CIS method with spin-orbit coupling

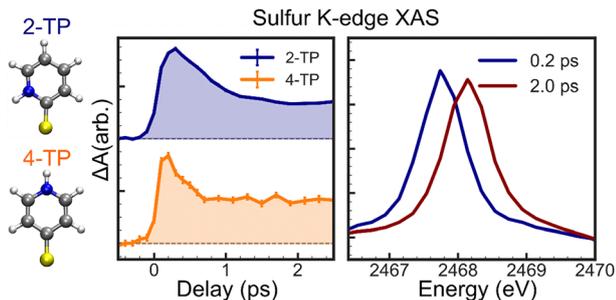
Aniket Mandal and John M. Herbert*

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Excited state dipole moments from Δ SCF: a benchmark

Lukas Paetow and Johannes Neugebauer*

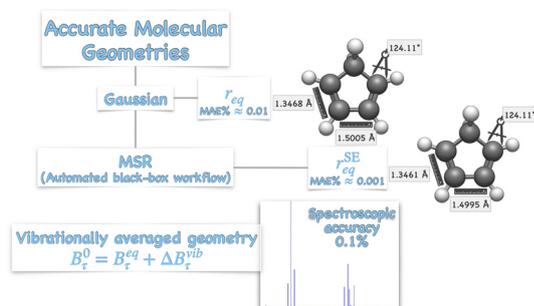
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Influence of substitution pattern on the dynamics of internal conversion and intersystem crossing in thiopyridone isomers

Douglas Garratt, Sambit K. Das, Kacie J. Nelson, Jessica Harich, Antonia Freibert, Camila Bacellar, Claudio Cirelli, Philip J. M. Johnson, Rebeca G. Castillo, Marija R. Zoric, Ru-Pan Wang, Hyeongtaek Lim, Amy A. Cordones, Nils Huse, Michael Odelius* and Kelly Gaffney*

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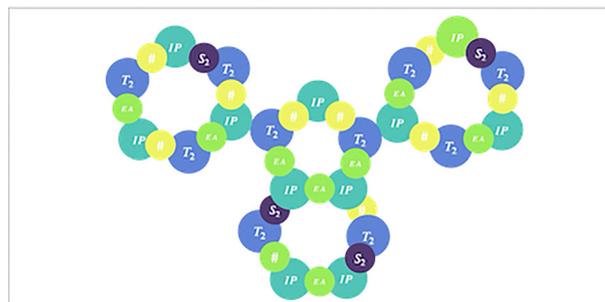
Computational efficiency meets spectroscopic accuracy: an unsupervised workflow for equilibrium geometries and vibrational effects in gas-phase prebiotic molecules

Marco Mendolicchio,* Lina Uribe, Federico Lazzari, Luigi Crisci, Giovanni Scalmani, Micheal J. Frisch and Vincenzo Barone*



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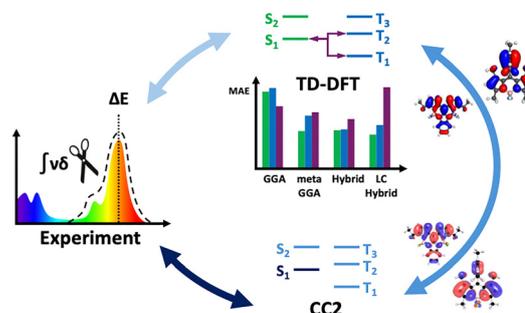
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Beyond the static picture: a machine learning and molecular dynamics insight on singlet fissionNatalia Szczepkowska, Iga Pręgowska,
Diana Radovanovici and Luis Enrique Aguilar Suarez*

16407

Investigating XC-functionals towards describing experimentally relevant excited-state properties of NIR-BODIPY derivatives

Mathias Fraiponts, Wouter Maes and Benoît Champagne*



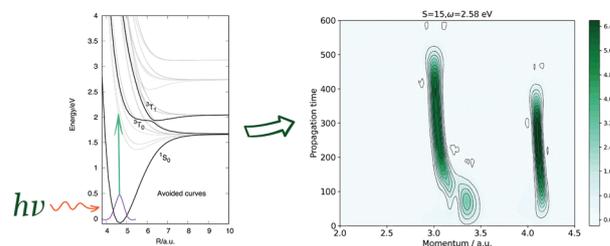
16418

Unitary coupled-cluster theory for the electron propagator: electron attachment and physical properties via the intermediate state representationManuel Hodecker, Andreas Dreuw and
Adrian L. Dempwolff*

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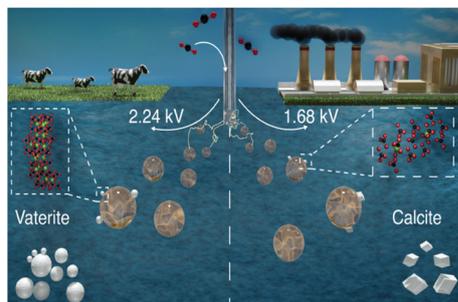
The strong-field control of IBr photodissociation re-visited

Cristina Sanz-Sanz* and Graham A. Worth



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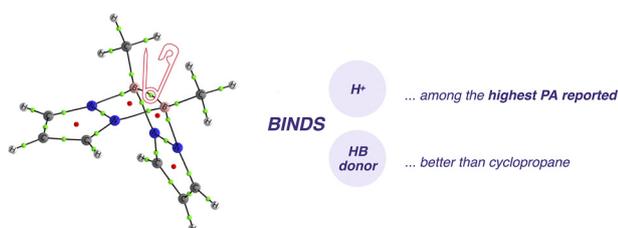
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Accelerated carbon dioxide mineralization and polymorphic control facilitated by nonthermal plasma bubbles

James Ho, Matthew Hershey and Dayne F. Swearer*

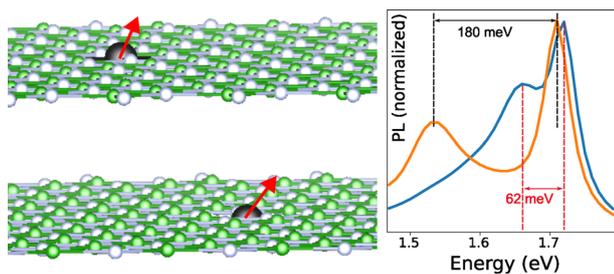
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Boron beats nitrogen: strained boron–boron bonds as (molecular) proton sponges

Ibon Alkorta,* José Elguero, M. Merced Montero-Campillo,* Otilia Mó and Manuel Yáñez

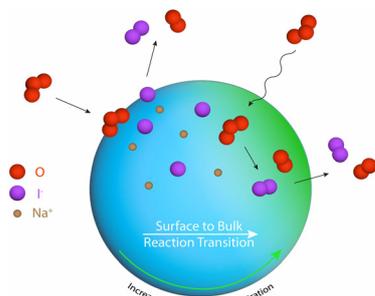
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Optical properties and spin states of inter-layer carbon defect pairs in hexagonal boron nitride: a first-principles study

Ignacio Chacon, Andrea Echeverri, Carlos Cardenas and Francisco Munoz*

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Surfactant control of interfacial reaction rates in aqueous microdroplets

Alexander M. Prophet, David T. Limmer and Kevin R. Wilson*

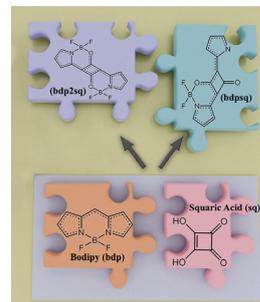


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Exploring the effect of squaraine infusion on the two-photon absorption cross-section of a few functionalized BODIPY-like systems

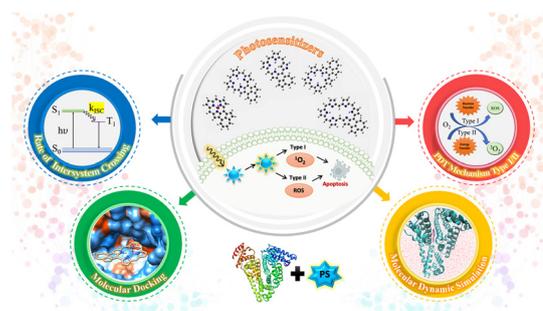
Tejendra Banana, Swati Singh Rajput, Neelam Chandravanshi and Md. Mehboob Alam*



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Designing expanded and contracted porphyrin–azulene based photosensitizers for photodynamic therapy

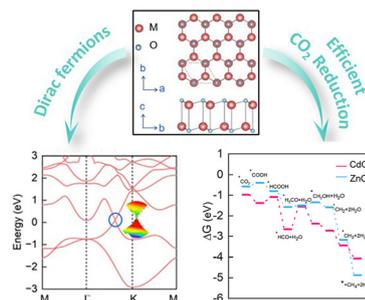
Swati Singh Rajput, Samarth Razdan, Tejendra Banana, Neelam Chandravanshi and Md. Mehboob Alam*



16498

Computational discovery of bilayer transition metal monoxides exhibiting Dirac fermions, superior carrier mobility, and efficient photocatalytic CO₂ reduction

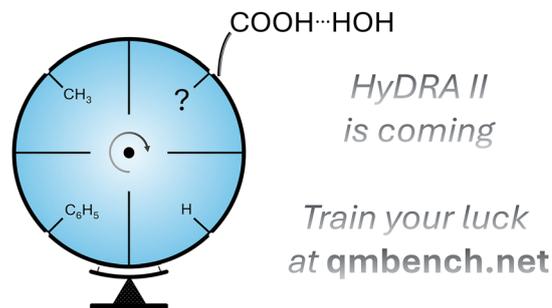
Rong Chen, Zhen Gao, Yang Liu, Keyi Song, Fengxian Ma and Yalong Jiao*



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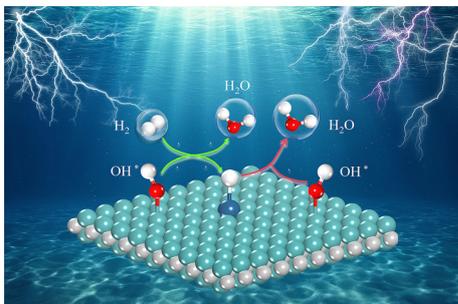
Vibrational signatures of carboxylic acid microhydration for the HyDRA project

Noah O. Evers, Sophie M. Schweer and Martin A. Suhm*



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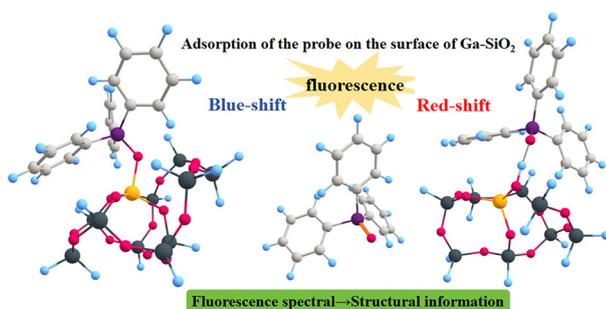
16518



Transition metal single-atoms anchored on Mo₂C MXenes for enhanced hydrogen oxidation reaction: a density functional theory study

Lianming Zhao,* Yizhu Wang, Tao Ding, Zeyue Peng, Zhumei Jiang, Jinghao Zhang, Xueru Wang, Yuan Li, Guang Zhao, Hao Ren, Wei Xing and Jing Xu*

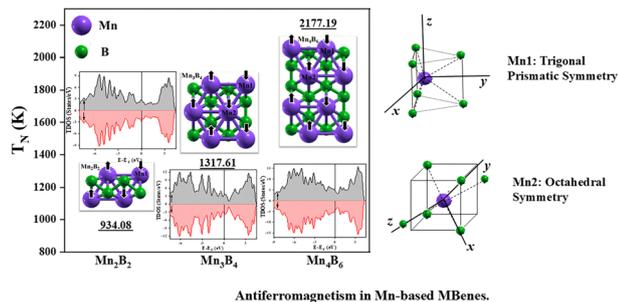
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Probing the adsorption behavior of triphenylphosphine oxide on the surface of Ga-SiO₂ with different binding sites

Yonggang Yang,* Chenhao Zheng, Yang Liu, Zhinan Jiang, Tiantian Guan, Chunsheng Zhuang* and Yufang Liu*

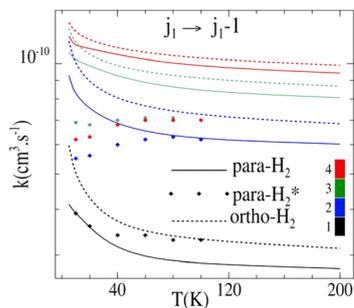
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Investigation of Mn-based MBenes towards the perspective of antiferromagnetic spintronics: a DFT study

Nayana Shekh and Alpa Dashora*

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New rate coefficients for rotationally inelastic collisions of OCS with *para*- and *ortho*-H₂

Samira Koudjeti, Haykel Elabidi, Fehmi Khadri, Kamel Hammami* and Nejmeddine Jaïdane

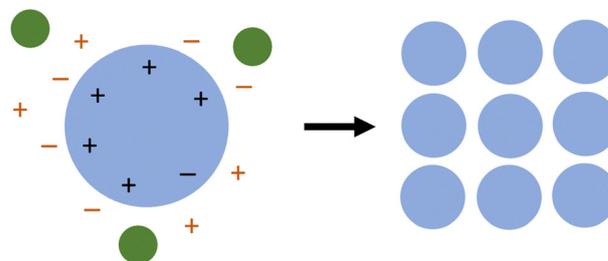


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Tailored solution environment for protein crystallization: tuning solubility, nucleation, and growth by urea and salt

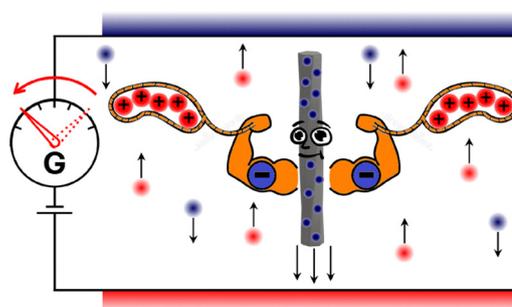
T. Hamacher and F. Platten*



16573

Conductometric evidence for accurate dissociation behaviour of surface groups on nanorods

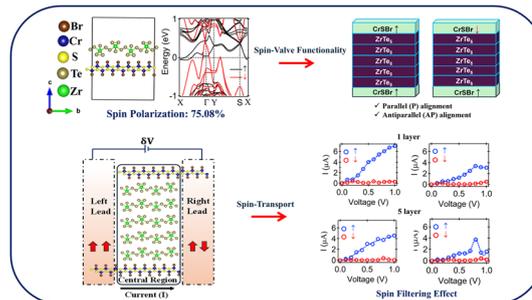
Marcel Kröger,* Kaarlo Nieminen, Han Tao and Eero Kontturi*



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Proximity-induced spin filtering in vdW CrSBr spin-valves with ZrTe₅ barriers

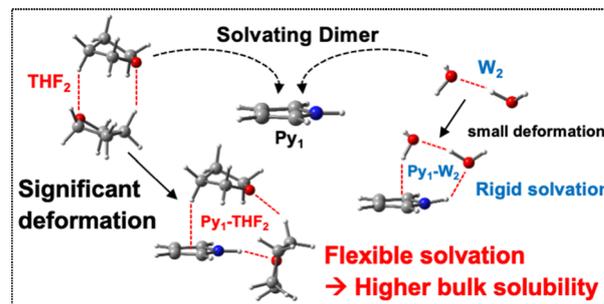
Puja Kumari, Anusree C V and V. Kanchana*



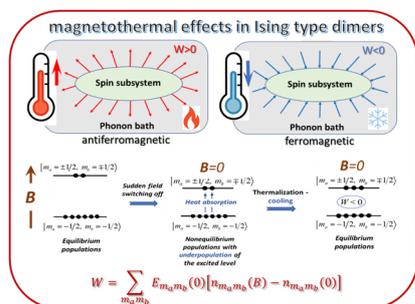
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Solvent-dimer-mediated clusters as a microscopic model of solution: IR spectroscopy and density functional theory of jet-cooled pyrrole-tetrahydrofuran clusters

Yoshiteru Matsumoto* and Yukino Yamada



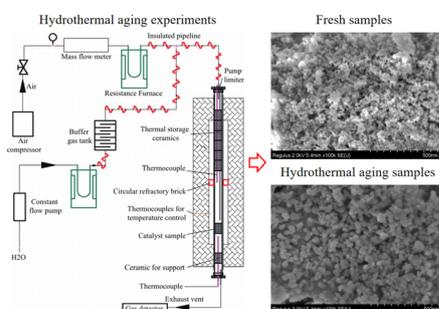
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Non-equilibrium magnetothermal effects in Ising dimers: relevance to the problem of low-temperature magnetic refrigeration

Andrew Palii,* Valeria Belonovich, Sergei Aldoshin and Boris Tsukerblat*

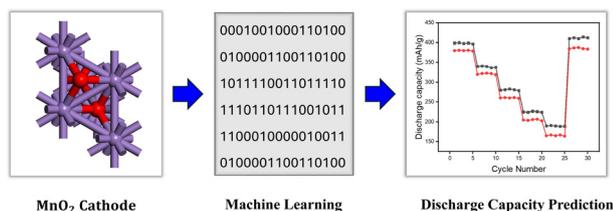
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Experimental and numerical studies on the hydrothermal aging stability and catalytic performance of three-way catalytic converters with different precious metal ratios and loading amounts

Zhen Gong, Tao Pan, Yejian Qian* and Wenxia Cao

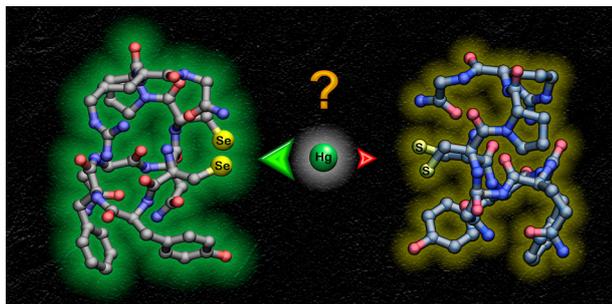
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Machine learning based prediction of MnO₂ cathode discharge capacity for high-performance zinc-ion batteries

Nure Alam Chowdhury, Leaford Nathan Adebayo Henderson, Samin Yaser, Olusola Pelumi Oyeku, Maydene Maydur Tresa, Chandra Kundu and Jayan Thomas*

16644



Shedding light on the HSAB-guided sulfur–selenium antagonism in mercury coordination and reactivity toward biologically relevant systems: a DFT and MD study

Pietro Delre, Ali Chahine, Giuseppe Felice Mangiatordi, Domenico Alberga, Michele Saviano, Germain Valverde, Luisa Ronga, Karinne Miqueu* and Panaghiotis Karamanis*

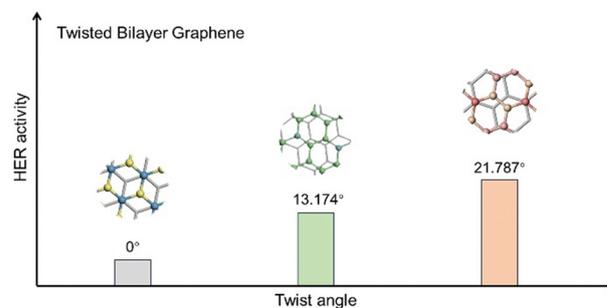


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Angle-dependent electrocatalytic activity of twisted bilayer graphene for the hydrogen evolution reaction

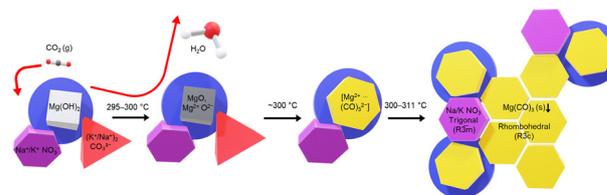
Lifang Chen, Jin Li and Xi Yin*



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Insights into the mechanism of nitrate salt-mediated MgCO₃ formation

Hellen Silva Santos,* Hoang Nguyen, Michael J. Bojdy, Pedram Esmaili, Juho Antti Sirviö and Paivo Kinnunen



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A novel non-Janus MoSF monolayer

Lin Zhang, Zhibin Gao, Longyuzhi Xu, Li Yang, Zhijing Huang,* Yuanbin Zhang,* Shuming Zeng* and Zonglin Gu*

