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Cover

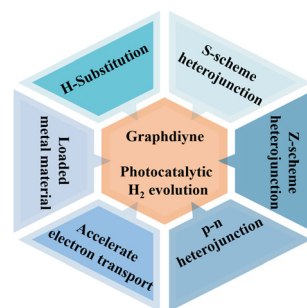
See Bikramjit Sharma et al., pp. 27879–27890.
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REVIEW

27846

Recent advances in graphdiyne for photocatalytic hydrogen evolution

Yu Fan, Xuqiang Hao* and Zhiliang Jin

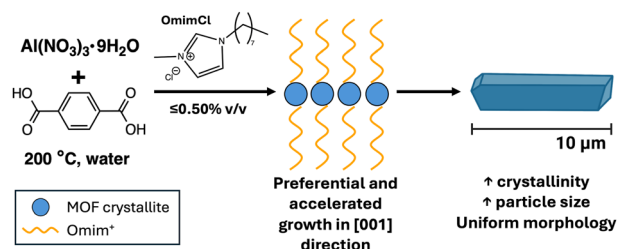


COMMUNICATIONS

27861

Influence of 1-methyl-3-octylimidazolium chloride on MIL-53(Al) crystallinity and particle size

Oliver Wang, Pranavsai Vadlamudi, Victoria Jang, Andrew Hoadley and Amnon G. Ortoll-Bloch*



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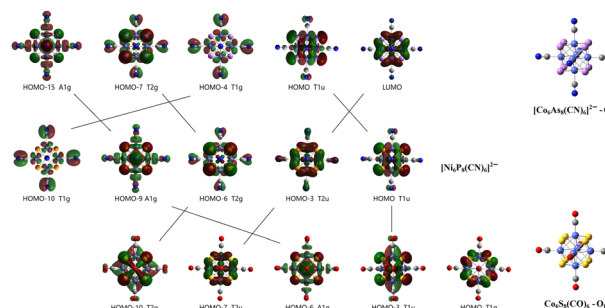


COMMUNICATIONS

27867

Extending the Chevrel-type superatoms to the nitrogen family

Ziyao Yang, Ning Du and Hongshan Chen*

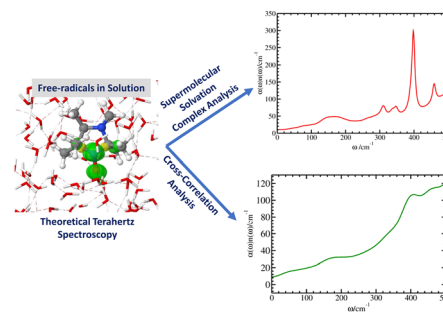


RESEARCH PAPERS

27879

Theoretical terahertz spectroscopy of free radical solutes in solution: an EPR spin probe in water

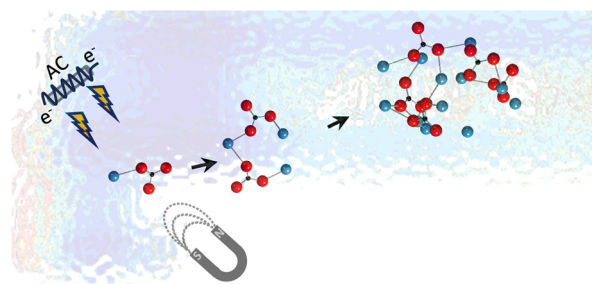
Bikramjit Sharma,* Philipp Schienbein, Harald Forbert and Dominik Marx



27891

Impact of magnetic and electric fields on the free energy to form a calcium carbonate ion-pair

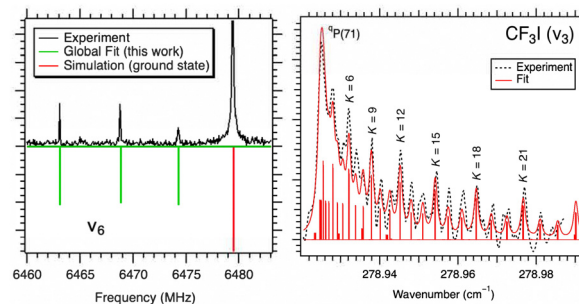
Ke Yuan,* Nikhil Rampal, Xuwei Du, Fangjun Shu, Yanxing Wang, Huiyao Wang, Andrew G. Stack, Paul Ben Ishai, Lawrence M. Anovitz and Pei Xu



27902

Reinvestigation of the ν_3 – ν_6 Coriolis interaction in trifluoroiodomethane

Arun Bhujel, Salma Akter, Muhammad Qasim Ali and G. Barratt Park*



RESEARCH PAPERS

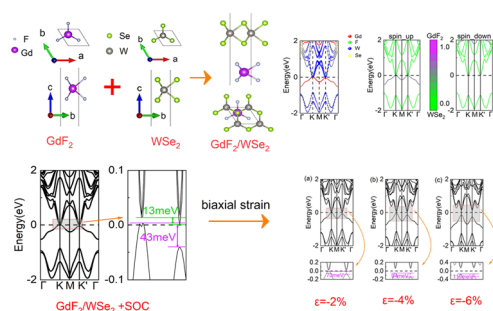
27912



IR spectra of cationic 1,5,9-triazacoronene and two of its cationic derivatives

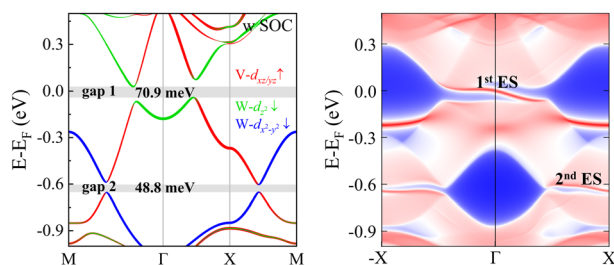
Jerry Kamer, Domenik Schleier, Andy Jiao, Grégory Schneider, Jonathan Martens, Giel Berden, Jos Oomens and Jordy Bouwman*

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Tunable valley polarization and high Curie temperature in two-dimensional $\text{GdF}_2/\text{WSe}_2$ van der Waals heterojunctions

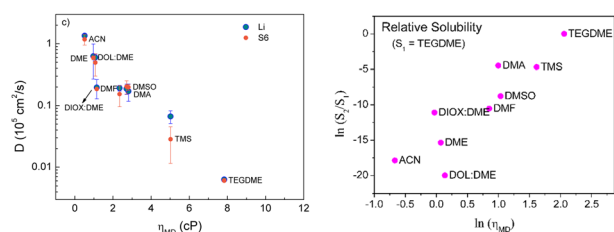
Xu Zhang, Kai Zhang, Yadong Zhu,* Baozeng Zhou* and Xiaocha Wang*

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Multi-level chiral edge states in Janus $\text{M}_2\text{XS}_2\text{Se}_2$ ($\text{M} = \text{V}, \text{Ti}$; $\text{X} = \text{W}, \text{Mo}$) monolayers with high Curie temperature and sizable nontrivial topological gaps

Li Deng, Xiang Yin, Yanzhao Wu, Junwei Tong, Gaowu Qin and Xianmin Zhang*

27945



Diffusion and thermodynamic properties of lithium polysulfides in different solvents: a molecular dynamics approach

Javier Luque Di Salvo,* Santiago Agustín Maldonado-Ochoa, Guillermina L. Luque, Andrea Calderón, Victoria Bracamonte, Fabián Vaca Chávez, Daniel E. Barraco, Alen Vizintin, Robert Dominko, Ezequiel P. M. Leiva* and Giorgio De Luca

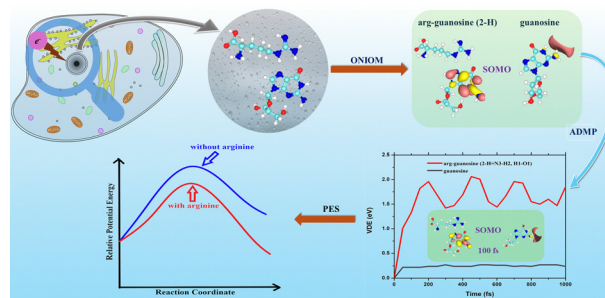


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Mechanistic insights into the electron attachment process to guanosine in the presence of arginine

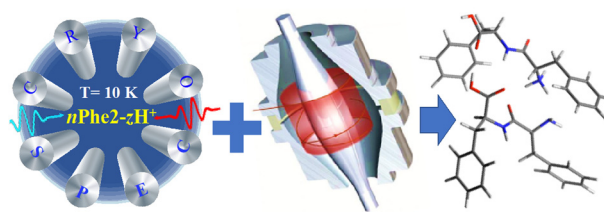
Manash Pratim Sarmah and Manabendra Sarma*



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Oligomers of diphenylalanine examined using cold ion spectroscopy and neural network-based conformational search

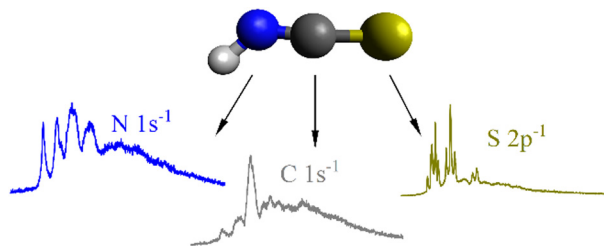
Vladimir Kopysov, Ruslan Yamaletdinov and Oleg V. Boyarkin*



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Experimental and theoretical investigation of the Auger electron spectra of isothiocyanic acid, HNCS

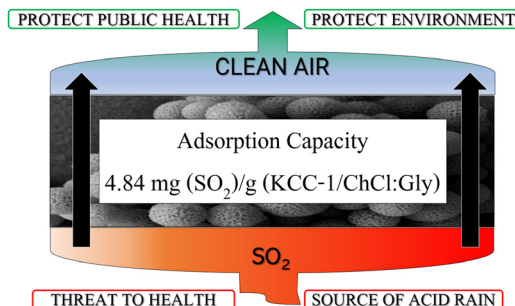
Dorothee Schaffner, Marius Gerlach, Emil Karaev, John Bozek, Ingo Fischer* and Reinhold F. Fink*



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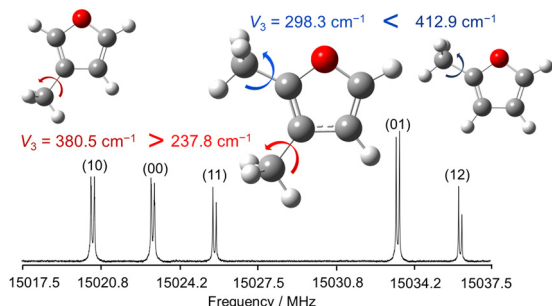
Dry desulphurisation of gas streams using KCC-1 mesoporous silica functionalised with deep eutectic solvents

Mohd Saiful Adli Azizman, Muhammad Adli Hanif, Naimah Ibrahim*, Ayu Wazira Azhari, Wan Khairunnisa Wan Ramli, Aishah Abdul Jalil, Nurul Sahida Hassan, Fazilah Farhana Abdul Aziz and Raja Nazrul Hakim Raja Nazri



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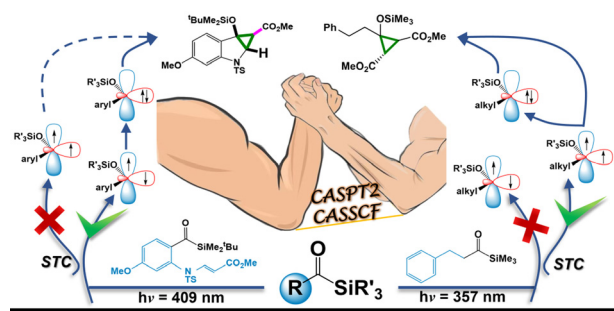
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Surprising torsional barrier reduction in the coupled methyl internal rotations of 2,3-dimethylfuran observed by microwave spectroscopy

Mike Buttkus-Barth, Thi Ha Nguyen, Gregor Brannys, Arne Lückow and Ha Vinh Lam Nguyen*

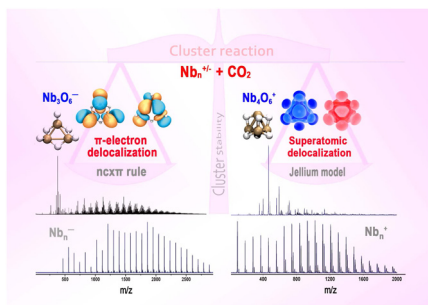
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Theoretical exploration of siloxy carbenes: photogeneration and [2+1] photocyclization mechanisms

Jianhao Li, Xiaohan Jiang, Zixi Liang, Chao Tang, Lishuang Ma,* Xufeng Lin, Xinmei Liu and Xuebo Chen

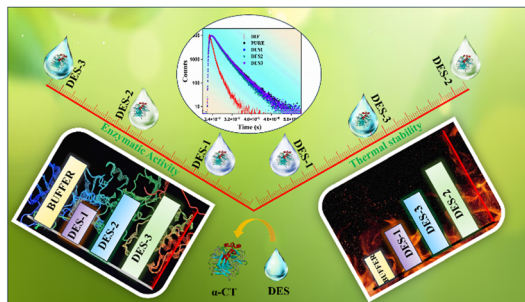
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Enhanced stability of the Nb_3O_6^- and Nb_4O_6^+ clusters: the $nxc\pi$ rule versus superatomic nature

Yifan Gao, Xin Lei, Ran Cheng, Shiquan Lin and Zhixun Luo*

28025



Unravelling the stabilization mechanism of mono-, di- and tri-cholinium citrate–ethylene glycol DESs towards α -chymotrypsin for preservation and activation of the enzyme

Bindu Yadav, Niketa Yadav and Pannuru Venkatesu*

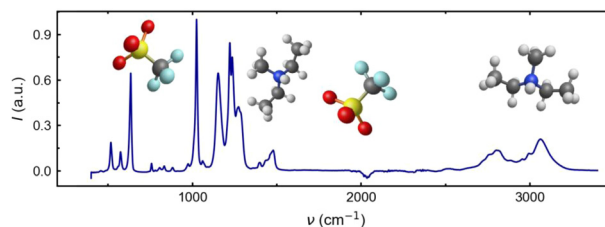


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Understanding the infrared spectrum of the protic ionic liquid [DEMA][TfO] by atomistic simulations

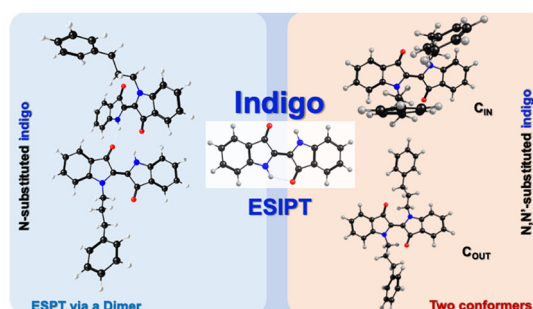
Federico Parisi, Yingzhen Chen, Klaus Wippermann, Carsten Korte, Piotr M. Kowalski, Michael Eikerling and Christian Rodenbücher*



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Solvent-dependent ultrafast deactivation processes with phenylpropyl indigo derivatives: a step forward in the understanding of indigo decay mechanisms

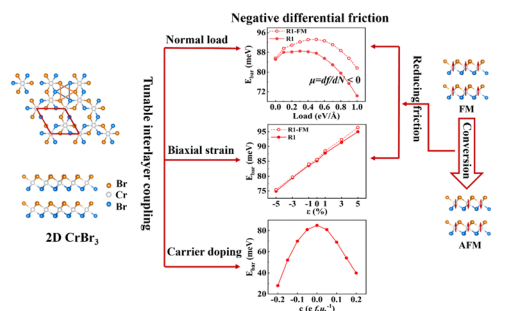
Daniela Pinheiro, Carla Cunha, Marta Pineiro, Adelino M. Galvão and J. Sérgio Seixas de Melo*



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Control of interlayer friction in two-dimensional ferromagnetic CrBr₃

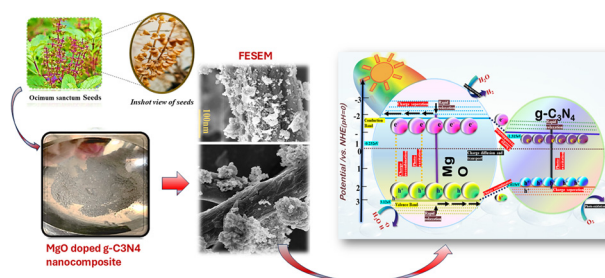
Xinyue Bi, Yushu Xu, Xinqi Zhang, Junqin Shi,* Tengfei Cao, Feng Zhou, Weimin Liu and Xiaoli Fan*



28064

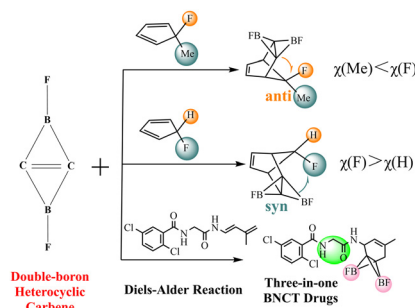
Eco-inspired synthesis of MgO-infused g-C₃N₄ nanocomposites from tulsi seeds for advanced photocatalytic environmental remediation

Sweeti Dahiya, Anshu Sharma and Sudesh Chaudhary*



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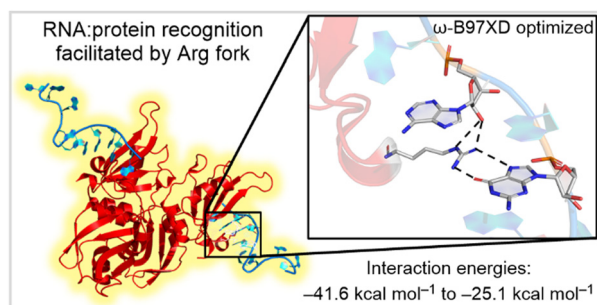
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Double-boron heterocyclic carbenes: a computational study of Diels–Alder reactions

Changyu Cao, Congjie Zhang,* Junjing Gu and Yirong Mo*

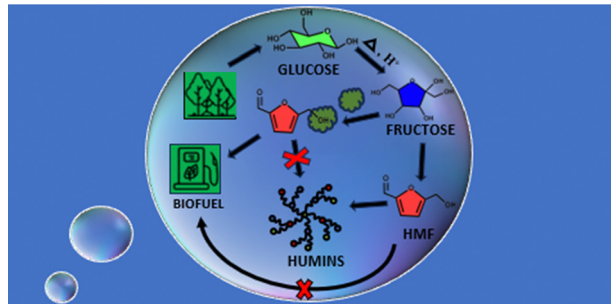
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Decoding the enigma of RNA–protein recognition: quantum chemical insights into arginine fork motifs

Raman Jangra, Teagan Kukhta, John F. Trant* and Purshotam Sharma*

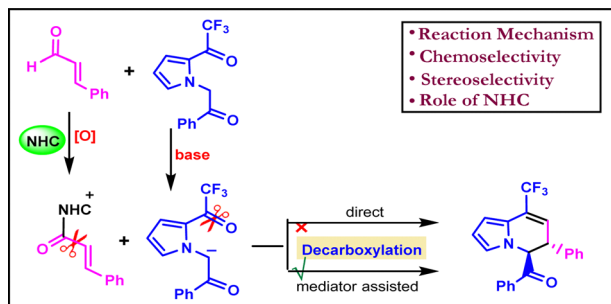
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Computational insights into selective glucose to 5-hydroxymethylfurfural (HMF) conversion by reducing humins formation in aqueous media under Brønsted acid-catalyzed conditions

Jogeswar Chhatra, Swetha Nair, Sankari Nattuvetty Sunil Kumar and Sooraj Kunnikuruvan*

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Mechanisms and origins of stereoselectivity in the NHC-catalyzed oxidative reaction of enals and pyrroles: a density functional theory study

Yan Li,* Mingchao Zhang and Zhiqiang Zhang*

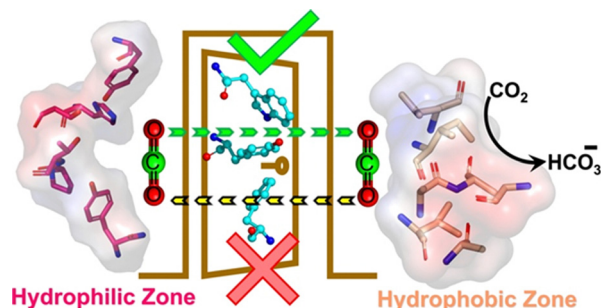


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Mechanism of a novel metal-free carbonic anhydrase

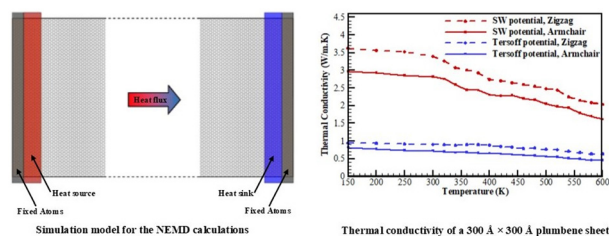
Shalini Yadav, Surajit Kalita* and Kshatresh Dutta Dubey*



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A molecular dynamics simulation study of thermal conductivity of plumbene

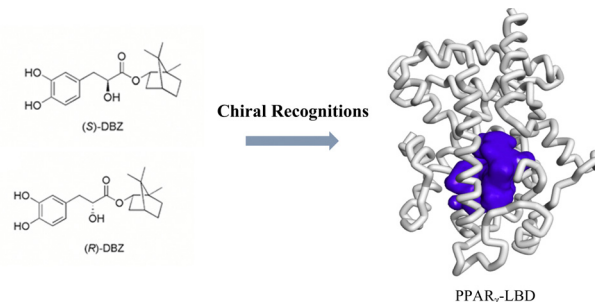
Rafat Mohammadi,* Behrad Karimi, John Kieffer and Daniel Hashemi



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Insights into the chirality-dependent recognition of Danshensu Bingpian Zhi stereoisomers with PPAR_γ

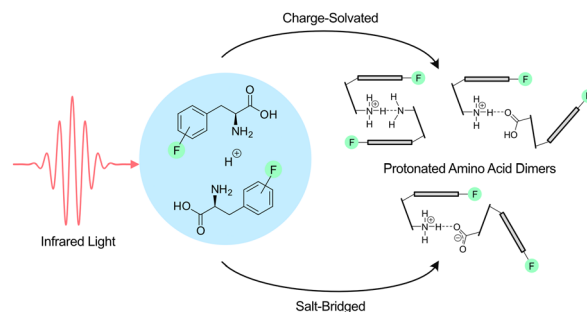
Jiasheng Zhao, Yizhen Zhao, Shengli Zhang, Lei Zhang and Zhiwei Yang*



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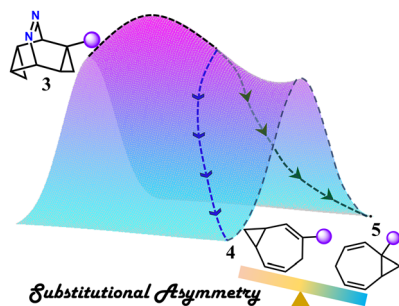
The impact of side-chain fluorination on proton-bound phenylalanine dimers: a cryogenic infrared spectroscopic study

Marc Safferthal, Kim Greis, Rayoon Chang, Chun-Wei Chang, Waldemar Hoffmann, Gerard Meijer, Gert von Helden and Kevin Pagel*



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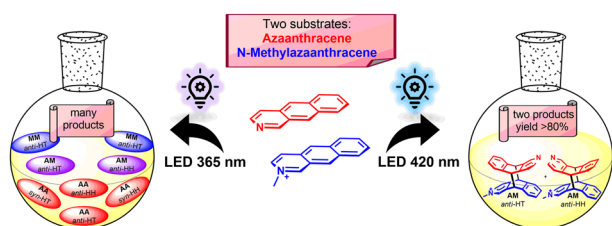
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Substitutional control of non-statistical dynamics in the thermal deazetization of tetracyclic azo compounds

Chandralekha Hajra and Ayan Datta*

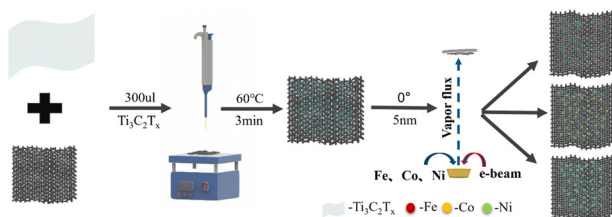
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Light-induced selectivity in an exemplary photodimerization reaction of varied azanthracenes

Adam Mames, Aleksander Gorski, Joanna Jankowska, Tomasz Ratajczyk* and Mariusz Pietrzak*

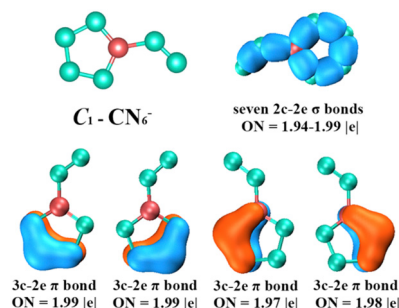
28182



Fe/Co/Ni modified $\text{Ti}_3\text{C}_2\text{T}_x$ nanosheets accelerate alkaline hydrogen evolution reaction

Yudong Xia,* Shujun Wu, Yifan Yan, Lingyu Liu, Fanggong Cai, Yuxiang Ni, Kai Ou* and Hongyan Wang

28191



Structural evolution and electronic properties of anionic carbon–nitrogen clusters

Yuanzhi Gao, Shu Huang, Peixin Fu, Chen Chen, Kewei Ding* and Cheng Lu*

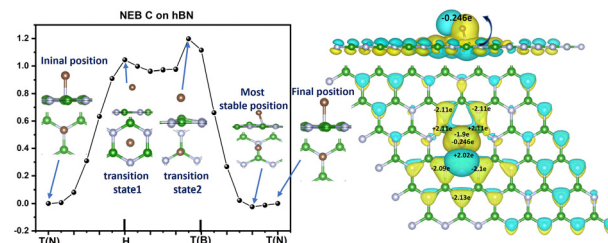


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Atomistic insights into the nucleation and growth of hexagonal boron nitride and graphene heterostructures

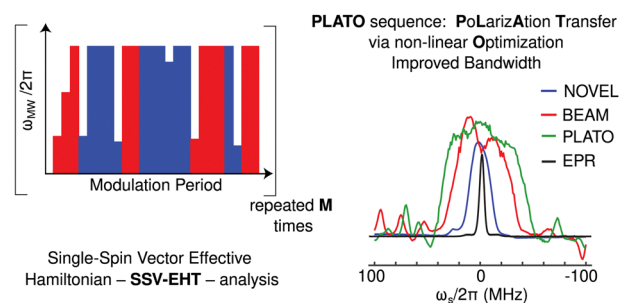
Mohamed Achehboune,* Kazem Zhour, Jaroslaw Dabrowski, Dominique Vignaud, Max Franck, Mindaugas Lukosius, Jean-François Colomer and Luc Henrard



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Dynamic nuclear polarization pulse sequence engineering using single-spin vector effective Hamiltonians

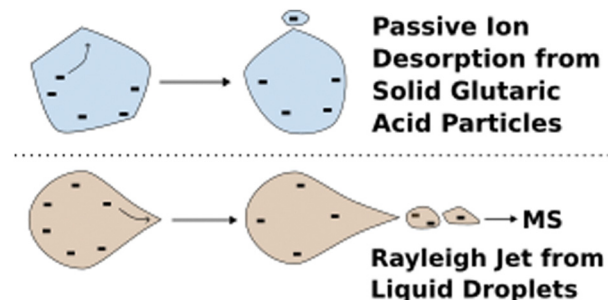
A. B. Nielsen, J. P. A. Carvalho, D. L. Goodwin, N. Wili and N. C. Nielsen*



28220

Modeling the ionization mechanism of amorphous solid particles without an external energy source coupled to mass spectrometry

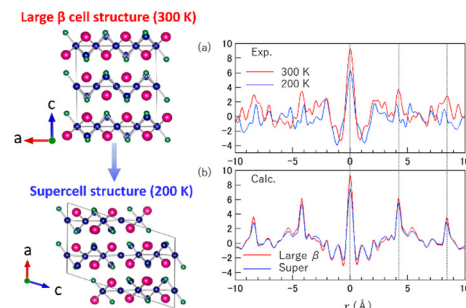
Styliani Consta,* Lisa M. Wingen, Yiming Qin, Veronique Perraud and Barbara J. Finlayson-Pitts



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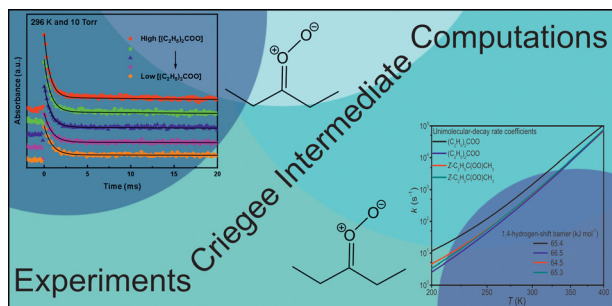
Structure of $\text{Bi}_2\text{Rh}_3\text{Se}_2$ above and below charge density wave transition determined by Bi $L\alpha$ and $L\gamma$ X-ray fluorescence holography

Zhiyan Zhang, Ritsuko Eguchi, Halubai Sekhar, Koji Kimura, Naohisa Happo, Yuki Yamamoto, Masaki Utsumi, Hidenori Goto, Koichi Hayashi and Yoshihiro Kubozono*



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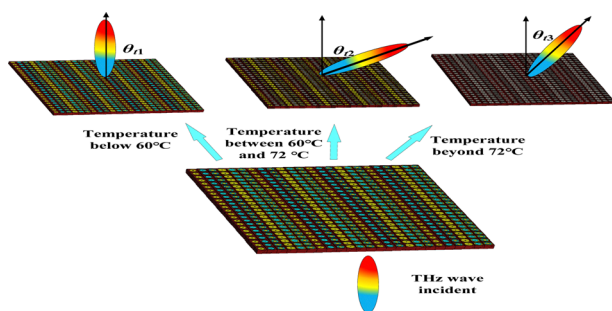
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An experimental and computational study of the unimolecular-decay reaction of diethyl-substituted Criegee intermediate ($(C_2H_5)_2COO$)

Jari Peltola, Timo T. Pekkanen, Petri Heinonen, Pyry Salomaa, Nino Runeberg, György Lendvay and Arkke J. Eskola*

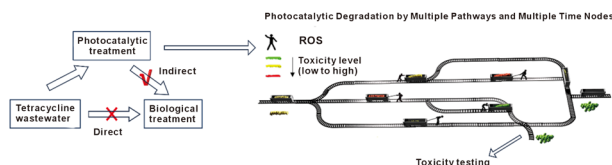
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A transmission-type terahertz beam reconfigurable metasurface based on a multilayer annular structure

Qi Chen, Junyi Yang, Jinqi Dong,* Lunyi Liu and Liang Liu

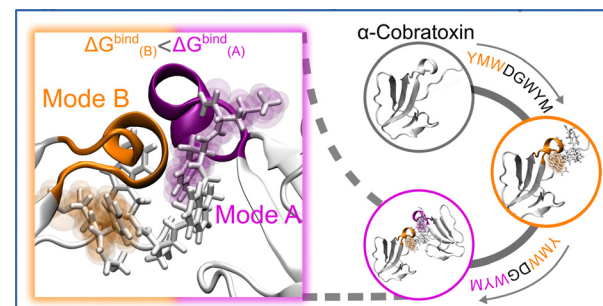
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Based on T.E.S.T toxicity prediction and machine learning to forecast toxicity dynamics in the photocatalytic degradation of tetracycline

Kaihang Liu, Wenhui Ni, Qiaoyu Zhang, Xu Huang, Tao Luo,* Jian Huang, Hua Zhang, Yong Zhang and Fumin Peng*

28274



Computational insight into the peptide-based inhibition of α -cobratoxin

Aritra Mitra, Viswas Pandijothi and Sandip Paul*



CORRECTION

28288

Correction: Supersolidity of undercoordinated and hydrating water

Chang Q. Sun

RETRACTION

28289

Retraction: Unprecedented O: $\leftrightarrow$:O compression and H $\leftrightarrow$ H fragilization in Lewis solutions

Chang Q. Sun

