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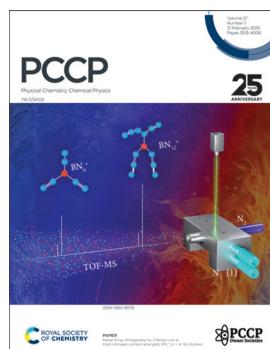
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See Hai-Feng Zhang et al.,
pp. 3558–3566.
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Inside cover

See Kewei Ding,
Hongguang Xu, Cheng Lu
et al., pp. 3567–3573.
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2025, 27, 3567.

EDITORIAL

3529

Festschrift for Judith Herzfeld: spectroscopic and theoretical studies of biomolecules, aqueous solutions, and materials

Ana-Nicoleta Bondar,* Leonid S. Brown,*
Hideki Kandori* and Vladimir Ladizhansky*



PERSPECTIVE

3531

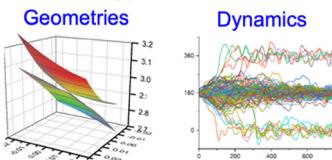
Analytical nuclear gradient and derivative coupling theories for multireference perturbation methods

Jae Woo Park

MRPT2 analytical gradients

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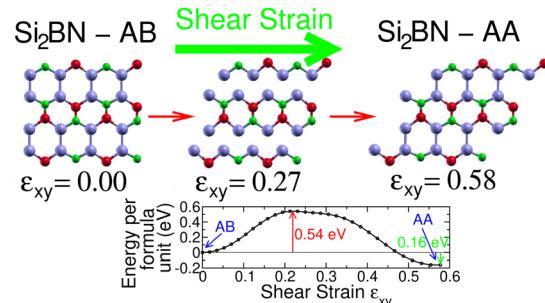


COMMUNICATION

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Unusual phase transition mechanism induced by shear strain in Si_2BN planar structures and comparison with graphene: an *ab initio* DFT study

Zacharias G. Fthenakis* and Madhu Menon*

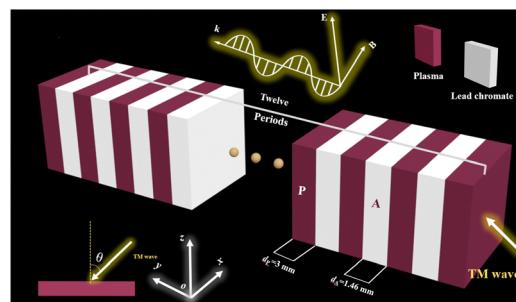


RESEARCH PAPERS

3558

An angle-selective photonic crystal for multi-physical sensing applications

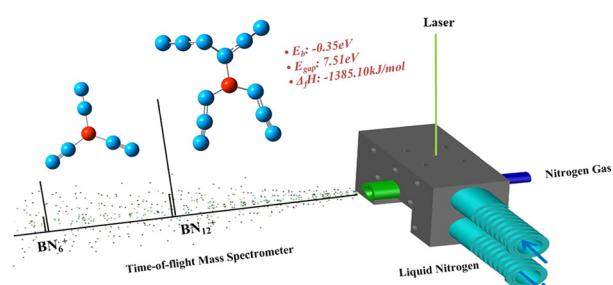
Na Pei, Bao-Fei Wan, Hao-Cheng Ma, Ting-Hao Zhang, Sen Hong and Hai-Feng Zhang*



3567

High-nitrogen-content energetic BN_n^+ ($n = 4\text{--}16$) clusters

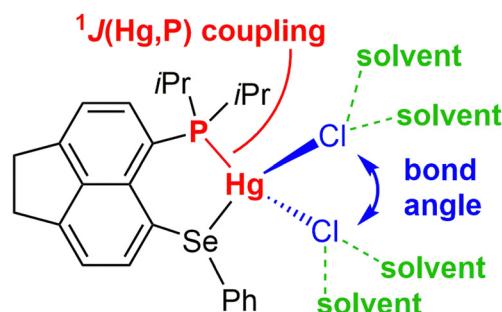
Jiale Li, Meicheng Chen, Kaiwen Liu, Kewei Ding,* Hongguang Xu,* Weijun Zheng and Cheng Lu*



3574

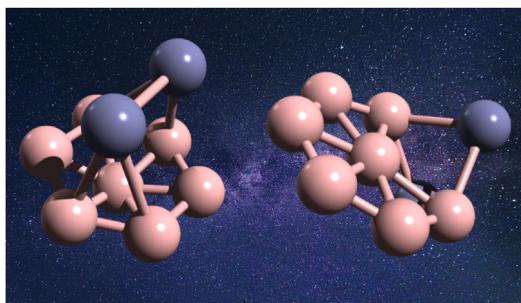
Investigation of the effect of solvation on ${}^1\text{J}(\text{Metal-P})$ spin–spin coupling

Olga L. Malkina,* Michael Bühl,* Brian A. Chalmers and S. Komorovsky



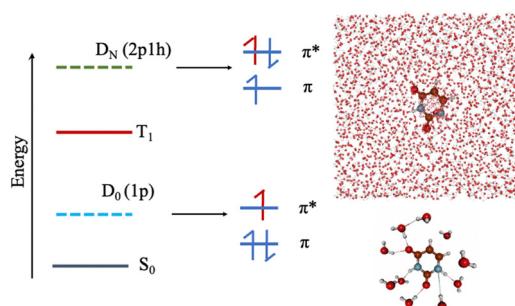
RESEARCH PAPERS

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**A Zn₂-supported B₇ wheel structure for the global minimum of the B₇Zn₂ cluster**

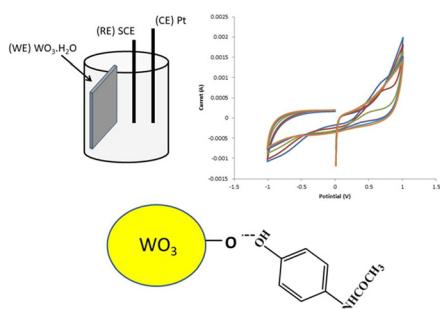
Peter L. Rodríguez-Kessler* and Alvaro Muñoz-Castro*

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**Impact of solvation on the electronic resonances in uracil**

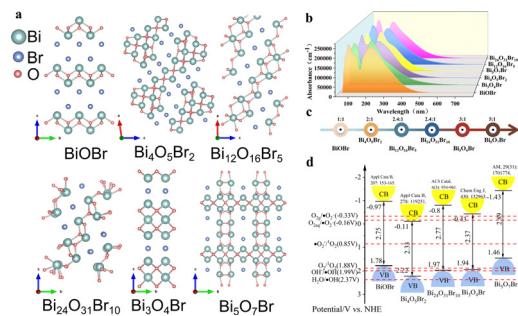
Divya Tripathi,* Maneesh Pyla, Achintya Kumar Dutta and Spiridoula Matsika*

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**A novel efficient electrochemical sensor for detecting paracetamol contaminants in polluted water using an active electrode from tungsten oxide nanoplates**

Reda Abdel-Hameed, Mohamed S. Elnouby,* Hoda F. Zahran, Nagah Abu-Rashed, Ashraf Ashmawy, Eshraqa Ali, Bader Huwaimel, M. Abdallah, Kaseb D. Alanazi, Elbadawy A. Kamoun* and Sara M. Younes

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Jing Zhang, Yang Liu, Shiheng Xin, Shihe Lin, Xin Zhang, Jiaxin Wang, Xiang Guo, Huichao Zhang, Ashish Kumar, Krishnamoorthy Ramachandran, Vadivel Subramaniam, Hongchao Ma,* Fuchun Zhang,* Qiang Zhang* and Xinghui Liu*

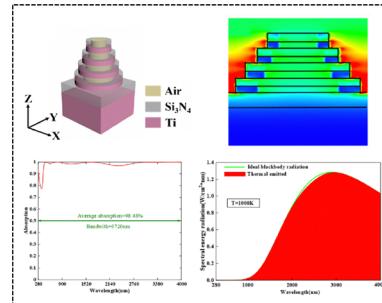


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An ultra-high absorptivity solar absorber with excellent thermal radiation efficiency based on a metal–dielectric stacked structure

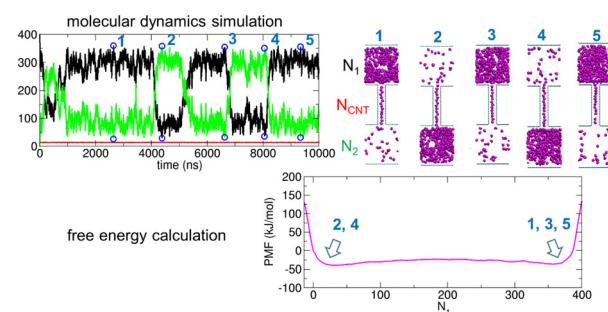
Yan Chen, Xiaoyun Wang, Sili Huang, Shiyi Song, Shanjun Chen,* Jie Hou and Yan Xiong



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Fluctuation-induced extensive molecular transport via modulation of interaction strength

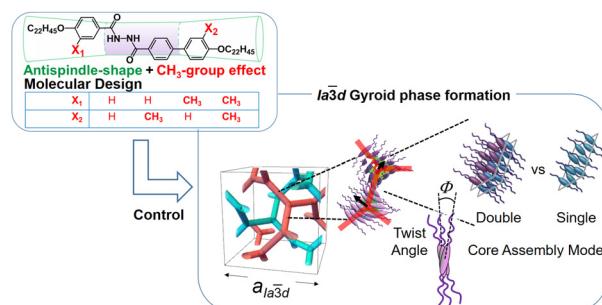
Changsun Eun



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Methyl side-groups control the $I\bar{a}3d$ phase in core-non-symmetric arylol-hydrazine-based molecules

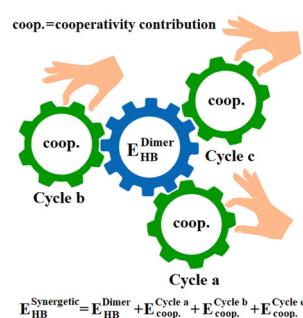
Sota Takebe, Nachia Isobe, Taro Udagawa, Yasuhisa Yamamura, Kazuya Saito, Yohei Miwa, Kei Hashimoto and Shoichi Kutsumizu*



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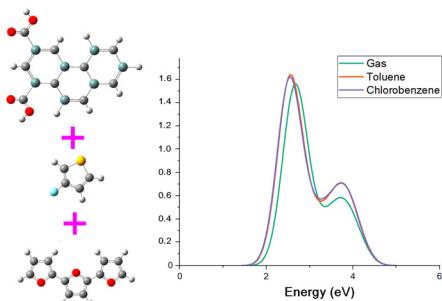
Cyclic cooperativity contributions determine the hydrogen bond strengths in molecular clusters

Ayush Shivhare, Bharti Dehariya, Shridhar R. Gadre and Milind M. Deshmukh*



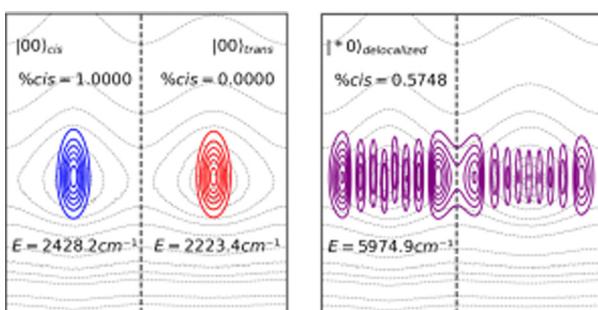
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**Enhancing organic SCs efficiency with CSi quantum dots in A- π -D architectures**

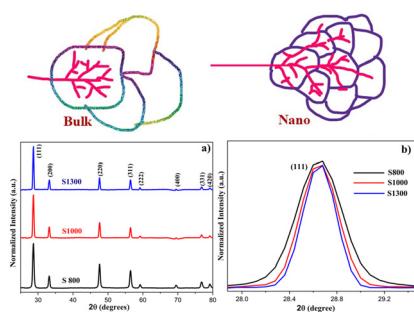
S. Insad, H. Ouarrad and L. B. Drissi*

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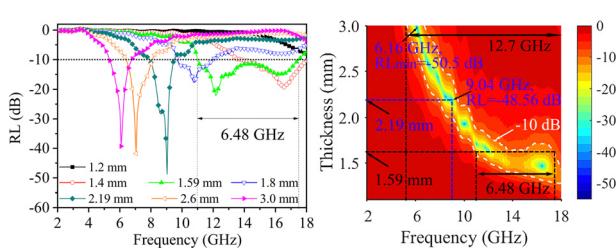
Leonardo J. Duarte,* Cláudio M. Nunes, Rui Fausto and Ataulpa A. C. Braga*

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**Higher stability of nanophase Gd_2O_3 – CeO_2 upon 400 keV Kr^+ ion irradiation over bulk: role of defect annealing across grain boundaries**

Waseem Ul Haq, V. Grover, Rakesh Shukla, Sanjay Kumar Kedia, Aman Singh, Sanjeev Kumar Srivastava, Shivam Shukla and Santanu Ghosh*

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**A novel cellulose-derived graphite carbon/ ZnO composite by atomic layer deposition as an over-wideband microwave absorber**

Guangguang Guan, Xiaojiang Li, Jiebai Li, Meng Chen, Hongpeng Liu, Wenbo Zhang, Jingyuan Wei and Yangtao Zhou*

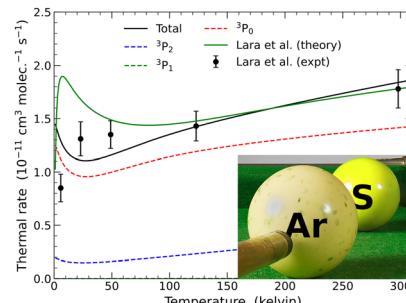


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Electronic quenching of sulfur induced by argon collisions

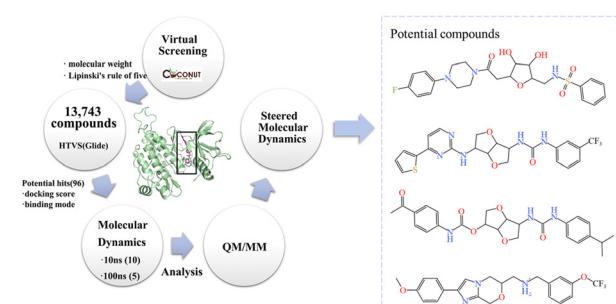
David M. G. Williams,* Nicole Weike, Manuel Lara, Kevin M. Dunseath and Alexandra Viel



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Discovery of potential VEGFR-2 inhibitors from natural products by virtual screening and molecular dynamics simulation

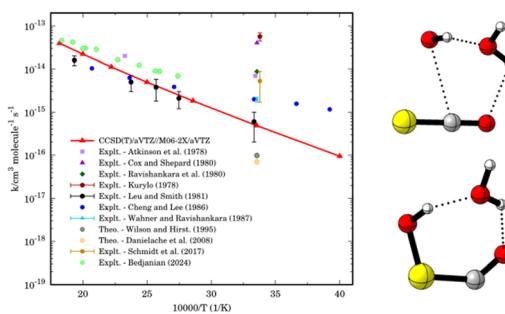
Qiong Xie, Mengshi Luo, Mingyan Liu, Yuxin Xie, Di Li, Hongjing Dai and Xiaohua Chen*



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Gas-phase and water-mediated mechanisms for the OCS + OH reaction

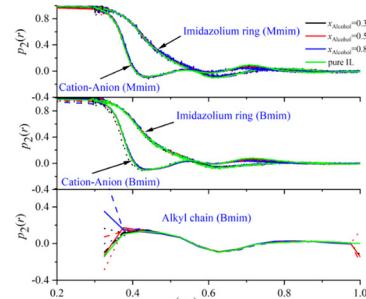
Joel Leitão Nascimento and Tiago Vinicius Alves*



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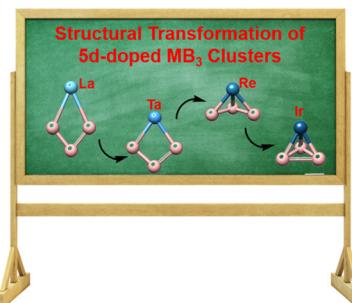
Molecular dynamics simulations of the structure and dynamics in mixtures of ionic liquids and alcohols

Farkhondeh Mozaffari



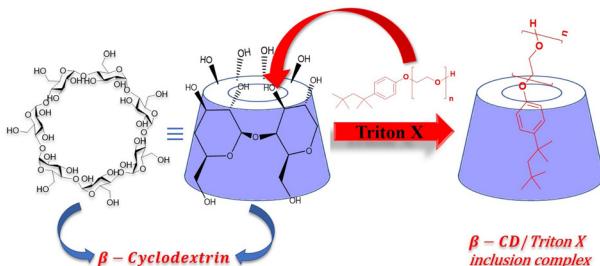
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**Probing the structural transformation and bonding of metal–boride clusters MB_3 ($\text{M} = \text{La}, \text{Ta}, \text{Re}, \text{Ir}$)**

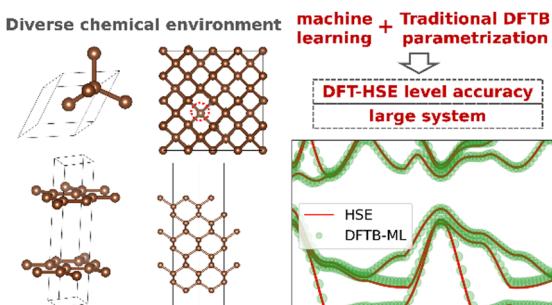
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**A physicochemical investigation of the complex formation by β -cyclodextrin with Triton X-100 and Triton X-114 and their aggregation behaviour in aqueous solution: an experimental approach**

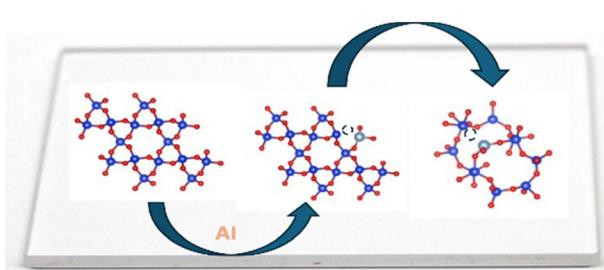
Rajesh Banik, Raju Sardar, Bipin Bihari Mondal and Soumen Ghosh*

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**Advancing band structure simulations of complex systems of C, Si and SiC: a machine learning driven density functional tight-binding approach**

Guozheng Fan, Yu Jing* and Thomas Frauenheim

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**Al doped silica glass: investigation of structural response and defect interactions based on crystalline models**

Astrid Marthinsen, Bartłomiej Adam Gaweł*, Gabriela Kazimiera Warden, Anna Górska - Ratusznik, Kamila Gaweł, Marisa Di Sabatino and Benny Hallam

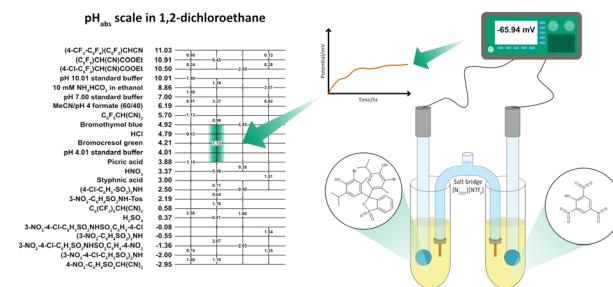


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Experimental unified pH scale in 1,2-dichloroethane

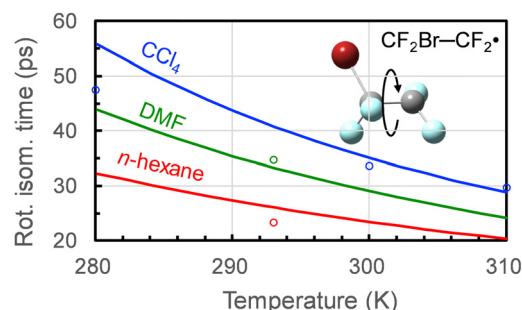
John Paulo Samin,* Agnes Heering, Jaan Saame,
Agnes Kütt and Ivo Leito*



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Determination of the rotational isomerization rate along carbon–carbon single bonds in solution

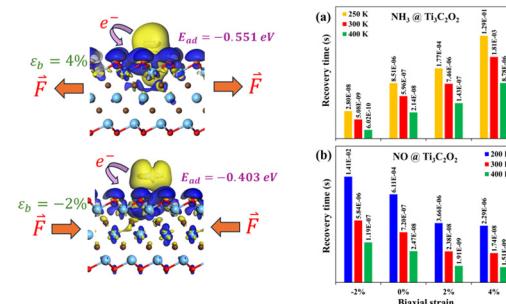
Seongchul Park, Hojeong Yoon, Juhyang Shin and
Manho Lim*



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Enhanced NH₃ and NO sensing performance of Ti₃C₂O₂ MXene by biaxial strain: insights from first-principles calculations

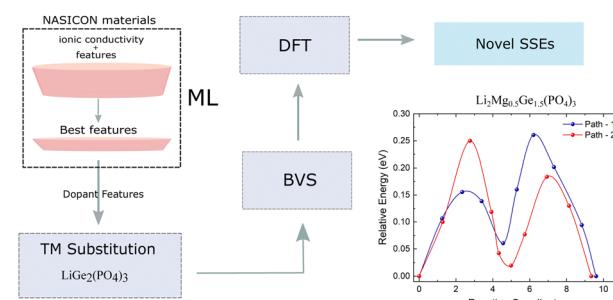
Satchakorn Khammuang, Kantaphong Wongphen,
Tanveer Hussain and Komsilp Kotmool*



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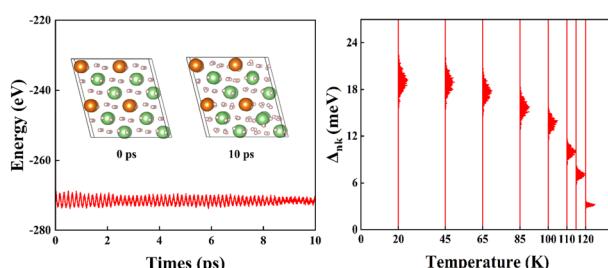
Accelerating discovery and design of high-performance solid-state electrolytes: a machine learning approach

Ram Sewak, Vishnu Sudarsanan and Hemant Kumar*



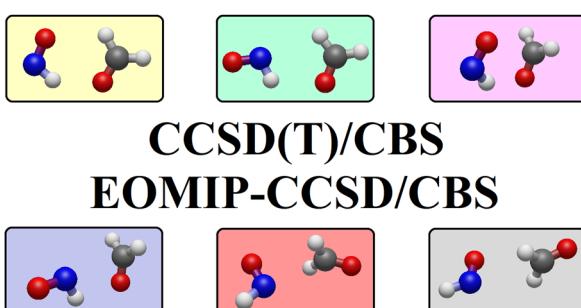
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**Stability and superconductivity of hexagonal prism-structured polyhydrides $X_2\text{MgH}_{18}$ ($X = \text{Li}, \text{Na}, \text{K}, \text{Rb}, \text{Cs}$) under moderate pressure**

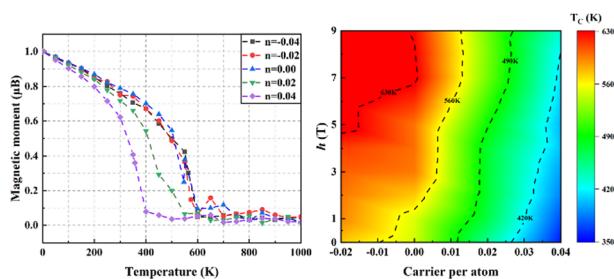
Liliang Zha, Jiajun Jiang, Yamin Xue, Zebang Cheng, Shunwei Yao, Wenjing Hu, Lin Peng,* Tingting Shi, Jing Chen, Xiaolin Liu and Jia Lin*

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**CCSD(T)/CBS
EOMIP-CCSD/CBS****Exploring ground-state and ionization potentials of the H₂CO...HNO dimers**

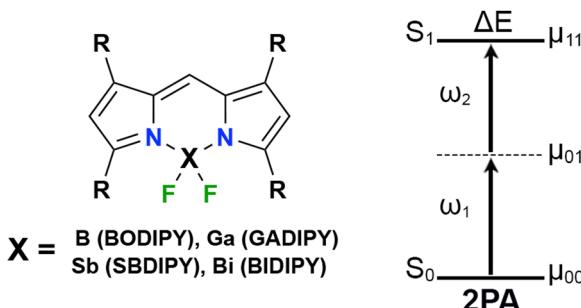
Gabriel L. C. de Souza* and Kirk A. Peterson*

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**The effect of carrier concentration on the electronic structure and magnetothermal properties of a two-dimensional VTe₂ monolayer with a high Curie temperature**

Shuai-Kang Zhang, Yan-Ling Wu, Zhao-Yi Zeng,* Hua-Yun Geng and Xiang-Rong Chen

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**Two-photon absorption of BODIPY, BIDIPY, GADIPY, and SBDIPY**

Ismael A. Elayan,* Mingmin Zhou and Alex Brown*

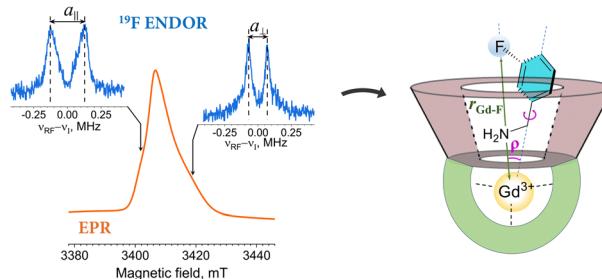


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Host–guest geometry in paramagnetic cavitands elucidated by ^{19}F electron-nuclear double resonance

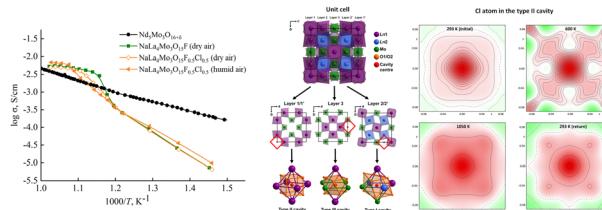
Alexey Bogdanov, Manas Seal, Elad Goren, Amnon Bar-Shir and Daniella Goldfarb*



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Structural features of sodium- and halogen-containing fluorite-like rare-earth molybdates

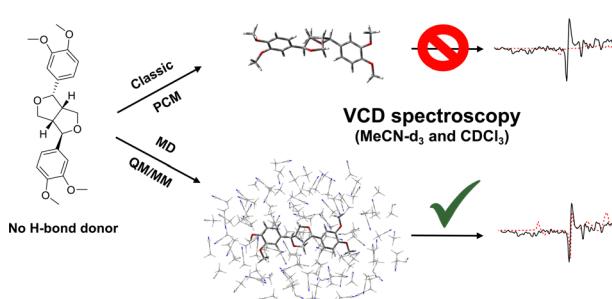
Alexander M. Antipin, Ekaterina I. Orlova,* Ekaterina S. Smirnova, Maria P. Trukhacheva, Timofei A. Sorokin, Ekaterina V. Sidorova, Elena P. Kharitonova, Nikolay V. Lyskov, Natalia E. Novikova,* Vasiliy O. Yapaskurt, Natalia I. Sorokina, Olga A. Alekseeva and Valentina I. Voronkova



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Solvent effects in furofuran lignans revealed by vibrational CD spectroscopy

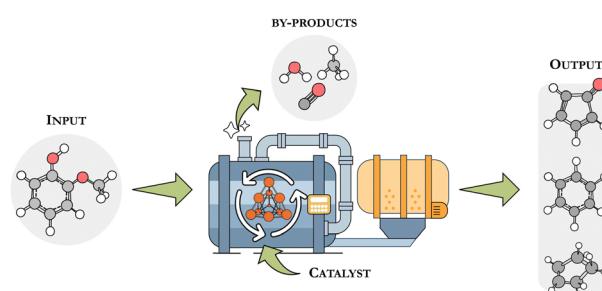
Eric Y. Lee, Victor M. S. Sousa, Eloá R. Mestriner, Kalil Bernardino, Isabele R. Nascimento* and João M. Batista Jr*



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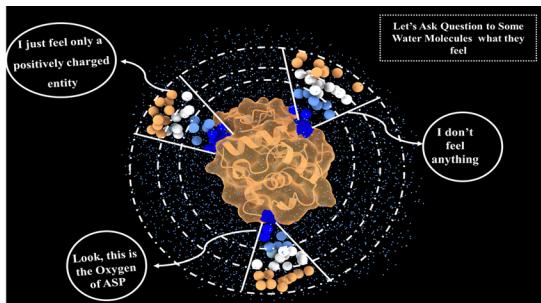
Decomposition of guaiacol on a subnanometric platinum cluster: a DFT investigation followed by microkinetic analysis

Chiara Nania, Francesco Ferrante,* Marco Bertini, Laura Gueci and Dario Duca



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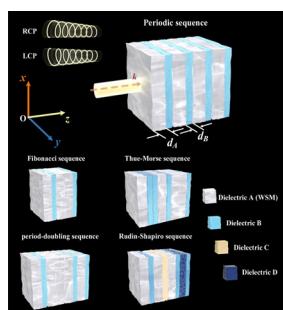
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Evaluating long-range orientational ordering of water around proteins: signature of a tug-of-war scenario

Subhabrata Hazra and Bimran Jana*

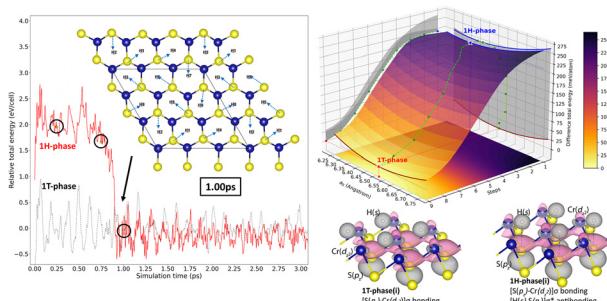
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Enhanced circular dichroism via multilayer Weyl semimetal material structures optimized with the Runge–Kutta algorithm

Jia-Tao Zhang, Ye Zheng and Hai-Feng Zhang*

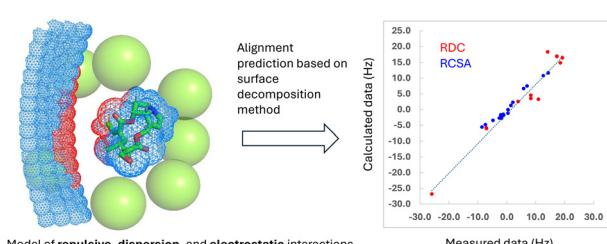
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Half-metallic and ferromagnetic phases in CrSH monolayers using DFT+U and BO-MD calculations

Akkarach Sukserm, Jakkapat Seeyangnok and Udomsilp Pinsook*

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A comprehensive solute–medium interaction model for anisotropic NMR data prediction

Yizhou Liu

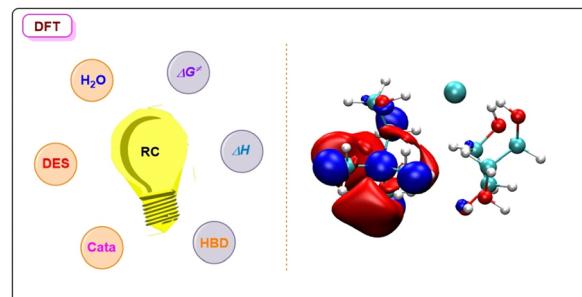


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Computational insights into asymmetric cross-alcohol carboligation in choline chloride/ethylene glycol deep eutectic solvents

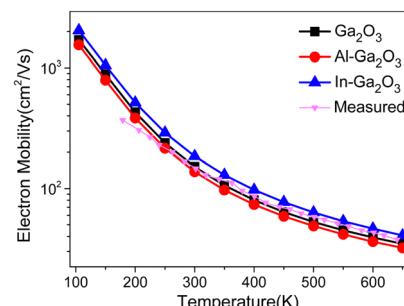
Yan Zhang, Yong Sheng Yang, Shi Jia Zhao, Cui Wei, Ning Zou,* Ying Xue* and Wen Jun Zhou*



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First principles investigation of electron mobility enhancement of $\beta\text{-Ga}_2\text{O}_3$ doped with indium

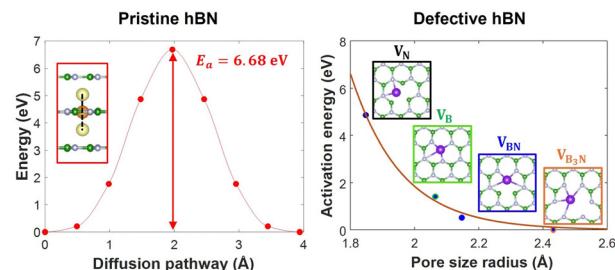
Leng Zhang,* Jiajian Huang, Yuhao Shen, Fei Liu, Pengzhan Zhang, Danbei Wang, Kongping Wu and Yaowei Wei



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First-principles elucidation of defect-mediated Li transport in hexagonal boron nitride

Yilong Zhou,* S. O. Kucheyev and Liwen F. Wan*



CORRECTIONS

4004

Correction: Structure, dynamic, and free energy analyses of 5-hydroxymethylfurfural in aprotic solvents and imidazolium ionic liquids using all-atom molecular dynamics simulations

Sweta Jha and Praveenkumar Sappidi*



CORRECTIONS

4006

Correction: Formulation and mechanism of copper tartrate – a novel anode material for lithium-ion batteries

Matthew Teusner, Uttam Mittal, Martina Lessio, Bernt Johannessen, Jitendra Mata and Neeraj Sharma*

