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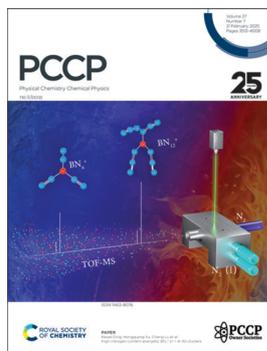
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Cover

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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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

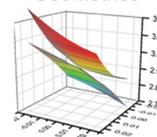
Jae Woo Park

MRPT2 analytical gradients

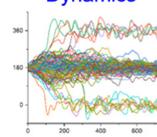
$$\frac{dE_{\text{MRPT2}}}{d\mathbf{R}} = \frac{\partial \mathcal{L}}{\partial \mathbf{R}}$$

Applications:

Geometries



Dynamics



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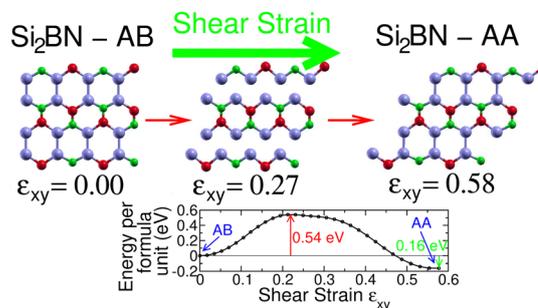
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COMMUNICATION

3552

Unusual phase transition mechanism induced by shear strain in Si₂BN planar structures and comparison with graphene: an *ab initio* DFT study

Zacharias G. Fthenakis* and Madhu Menon*

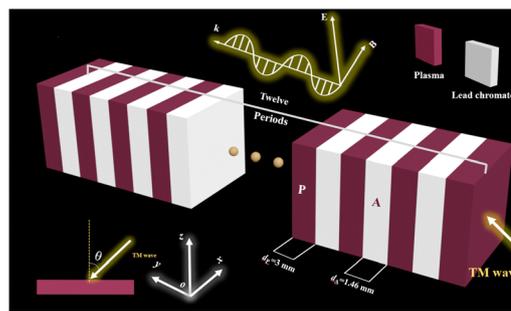


RESEARCH PAPERS

3558

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

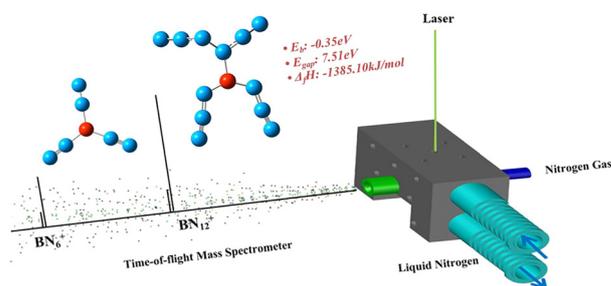
Na Pei, Bao-Fei Wan, Hao-Cheng Ma, Ting-Hao Zhang, Sen Hong and Hai-Feng Zhang*



3567

High-nitrogen-content energetic BN_n⁺ (n = 4–16) clusters

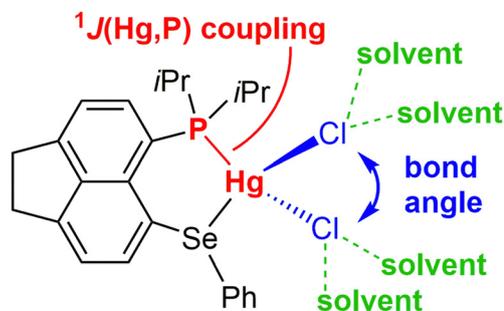
Jiale Li, Meicheng Chen, Kaiwen Liu, Kewei Ding,* Hongguang Xu,* Weijun Zheng and Cheng Lu*



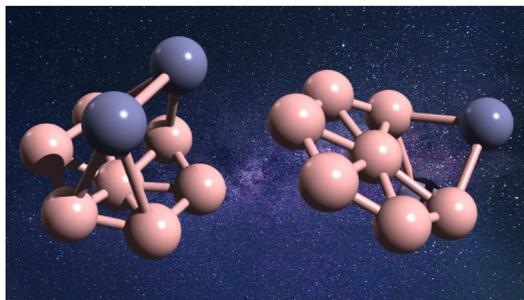
3574

Investigation of the effect of solvation on ¹J(Metal–P) spin–spin coupling

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



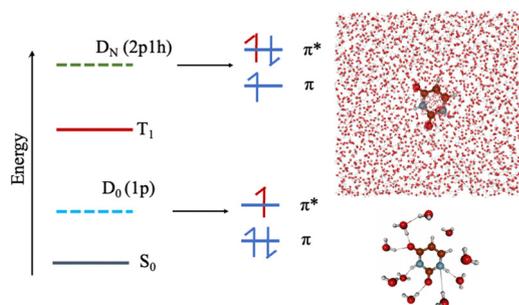
3583



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

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

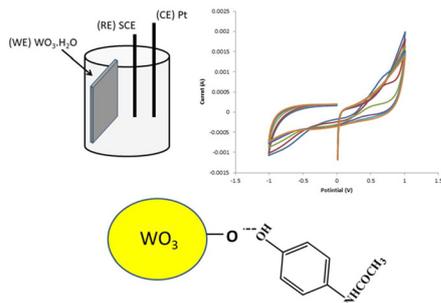
3588



Impact of solvation on the electronic resonances in uracil

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

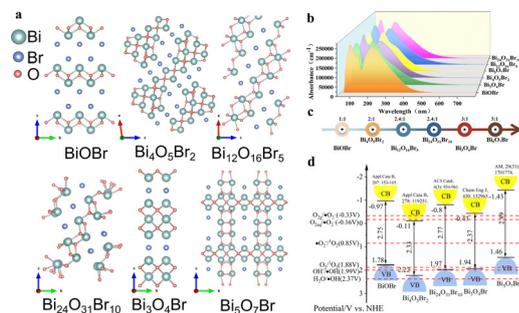
3602



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

3612



First-principles study of the effect of Bi content on the photocatalytic performance of bismuth bromide oxide-based catalysts

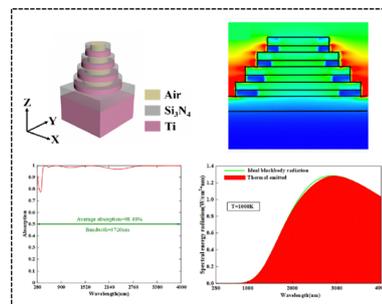
Jing Zhang, Yang Liu, Shiheng Xin, Shihe Lin, Xin Zhang, Jiaxin Wang, Xiang Guo, Huichao Zhang, Ashish Kumar, Krishnamoorthy Ramachandran, Vadivel Subramaniam, Hongchao Ma,* Fuchun Zhang,* Qiang Zhang* and Xinghui Liu*



3622

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

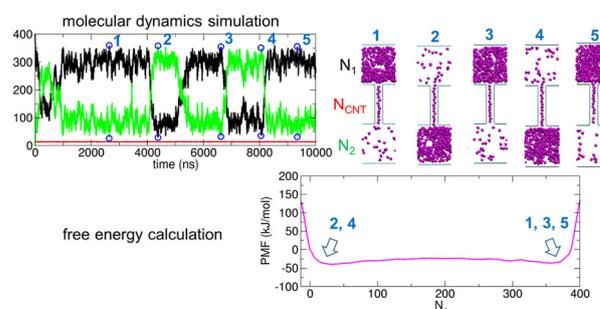
Yan Chen, Xiaoyun Wang, Sili Huang, Shiyi Song, Shanjun Chen,* Jie Hou and Yan Xiong



3634

Fluctuation-induced extensive molecular transport via modulation of interaction strength

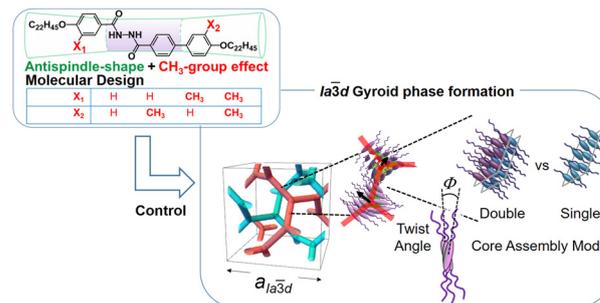
Changsun Eun



3650

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

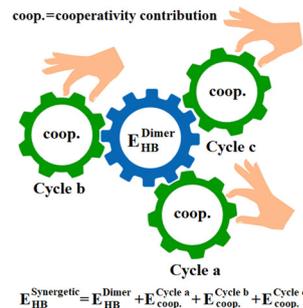
Sota Takebe, Nachia Isobe, Taro Udagawa, Yasuhisa Yamamura, Kazuya Saito, Yohei Miwa, Kei Hashimoto and Shoichi Kutsumizu*



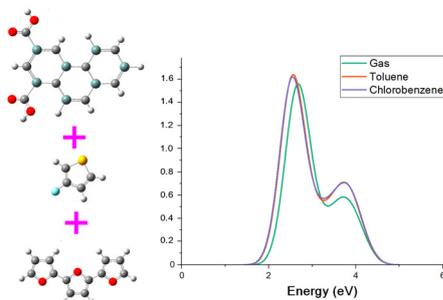
3661

Cyclic cooperativity contributions determine the hydrogen bond strengths in molecular clusters

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



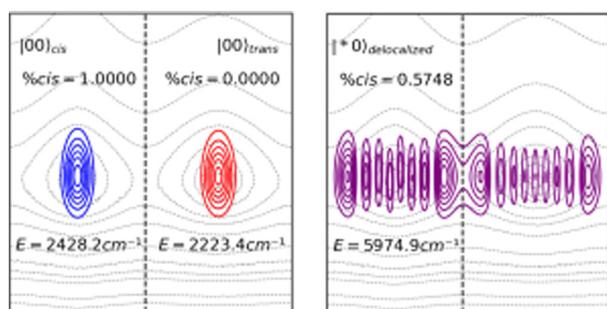
3673



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

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

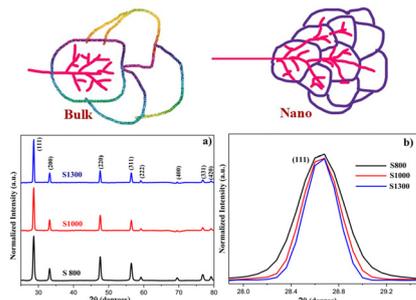
3685



A protocol for the investigation of the intramolecular vibrational energy redistribution problem: the isomerization of nitrous acid as a case of study

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

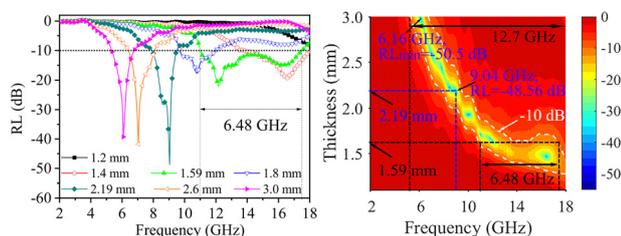
3701



Higher stability of nanophase Gd₂O₃-CeO₂ 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*

3715



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

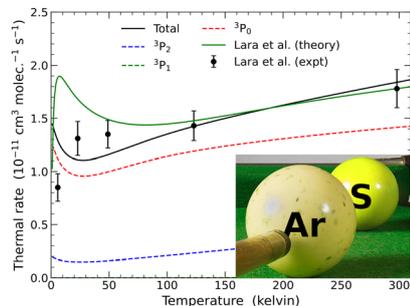
Guangguang Guan, Xiaoqiang Li, Jiebai Li, Meng Chen, Hongpeng Liu, Wenbo Zhang, Jingyuan Wei and Yangtao Zhou*



3722

Electronic quenching of sulfur induced by argon collisions

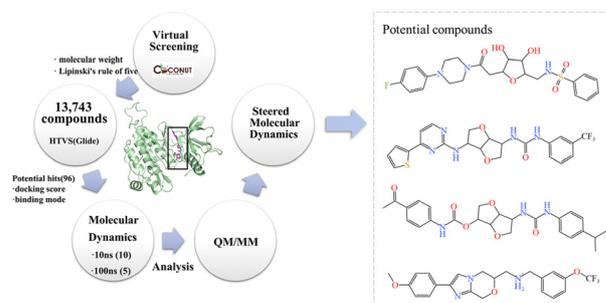
David M. G. Williams,* Nicole Weike, Manuel Lara, Kevin M. Dunseath and Alexandra Viel



3732

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

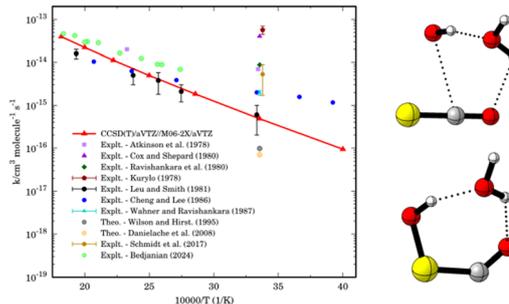
Qiong Xie, Mengshi Luo, Mingyan Liu, Yuxin Xie, Di Li, Hongjing Dai and Xiaohua Chen*



3748

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

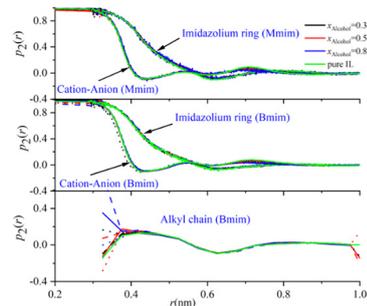
Joel Leitão Nascimento and Tiago Vinicius Alves*



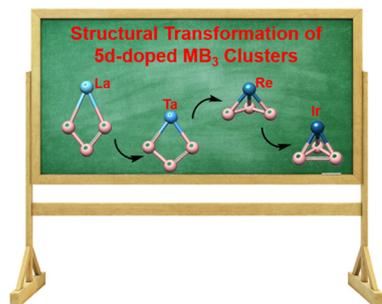
3755

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

Farkhondeh Mozaffari



3773



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

Xue-Lian Jiang, Xin-Ran Dong, Cong-Qiao Xu* and Jun Li*

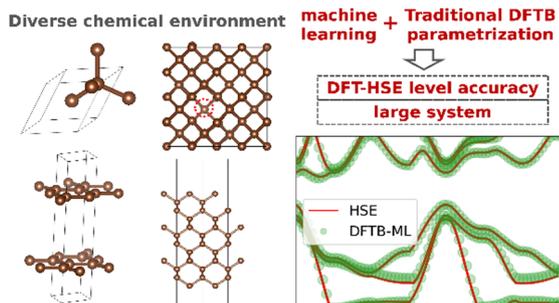
3782



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*

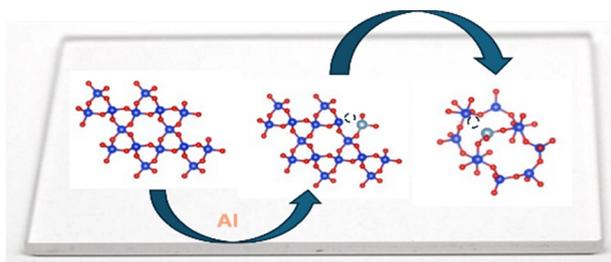
3796



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

3803



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

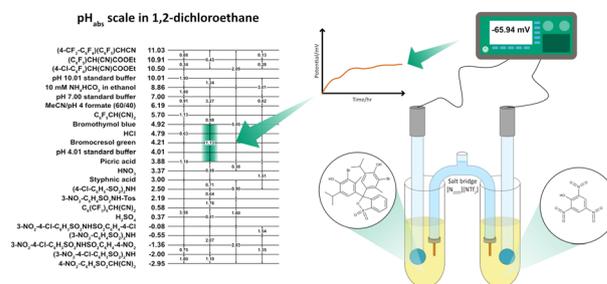
Astrid Marthinsen, Bartłomiej Adam Gawet*, Gabriela Kazimiera Warden, Anna Górska - Ratusznik, Kamila Gawet, Marisa Di Sabatino and Benny Hallam



3810

Experimental unified pH scale in 1,2-dichloroethane

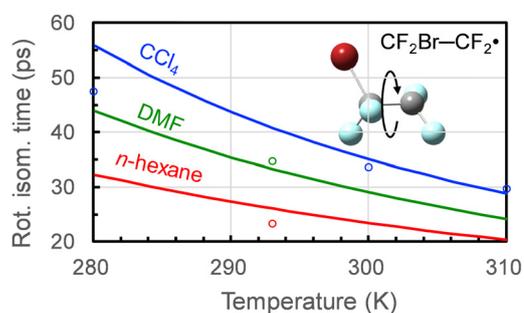
John Paulo Samin,* Agnes Heering, Jaan Saame, Agnes Kütt and Ivo Leito*



3817

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

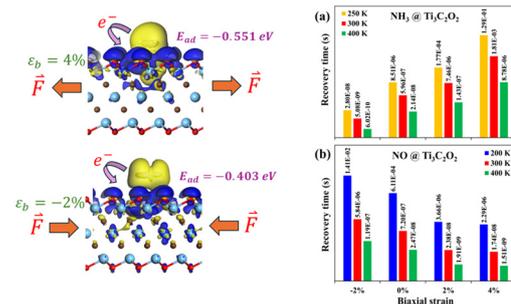
Seongchul Park, Hojeong Yoon, Juhyang Shin and Manho Lim*



3827

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

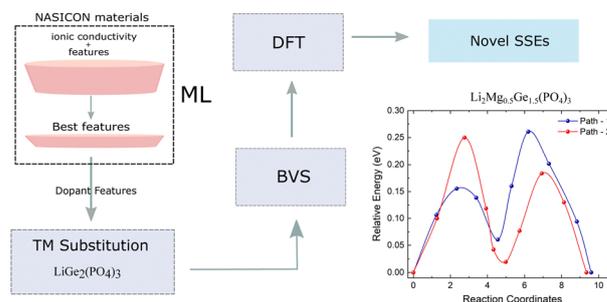
Satchakorn Khammuang, Kantaphong Wongphen, Tanveer Hussain and Komsilp Kotmoot*



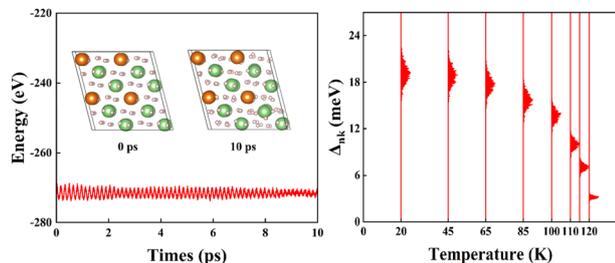
3834

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

Ram Sewak, Vishnu Sudarsanan and Hemant Kumar*



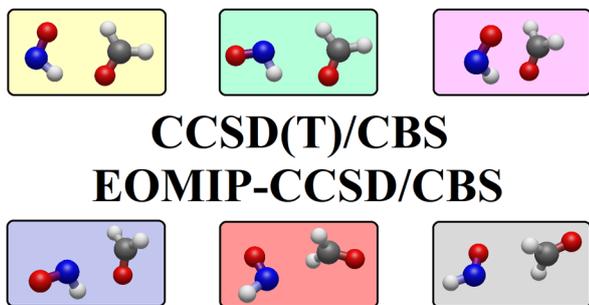
3844



Stability and superconductivity of hexagonal prism-structured polyhydrides X_2MgH_{18} ($X = Li, Na, K, Rb, Cs$) 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*

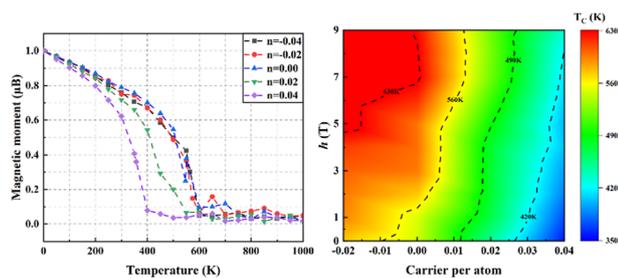
3854



Exploring ground-state and ionization potentials of the $H_2CO \cdots HNO$ dimers

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

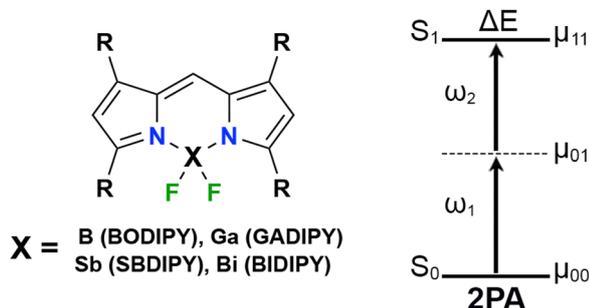
3861



The effect of carrier concentration on the electronic structure and magnetothermal properties of a two-dimensional VTe_2 monolayer with a high Curie temperature

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

3873



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

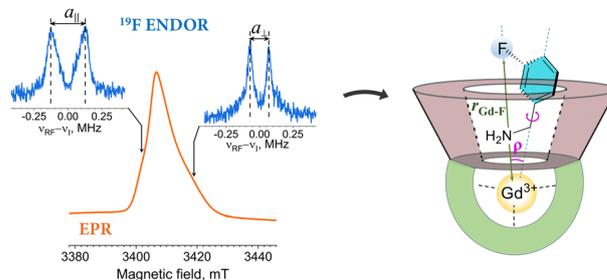
Ismael A. Elayan,* Mingmin Zhou and Alex Brown*



3885

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

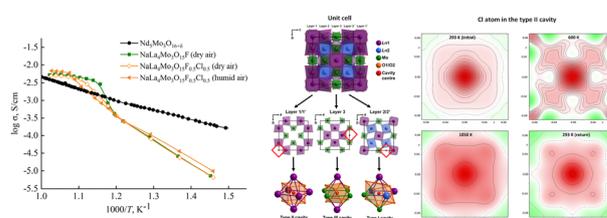
Alexey Bogdanov, Manas Seal, Elad Goren, Amnon Bar-Shir and Daniella Goldfarb*



3897

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

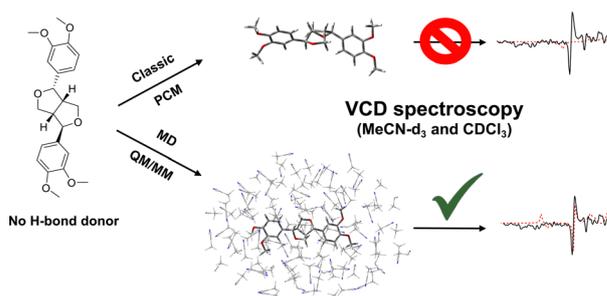
Alexander M. Antipin, Ekaterina I. Orlova,* Ekaterina S. Smirnova, Maria P. Trukhacheva, Timofei A. Sorokin, Ekaterina V. Sidorova, Elena P. Kharitonova, Nikolay V. Lyskov, Natalia E. Novikova,* Vasilij O. Yapaskurt, Natalia I. Sorokina, Olga A. Alekseeva and Valentina I. Voronkova



3908

Solvent effects in furofuran lignans revealed by vibrational CD spectroscopy

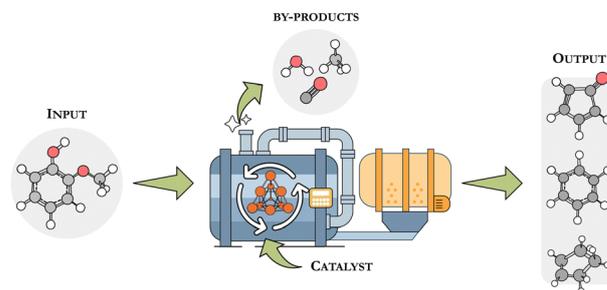
Eric Y. Lee, Victor M. S. Sousa, Eloá R. Mestriner, Kalil Bernardino, Isabele R. Nascimento* and João M. Batista Jr*



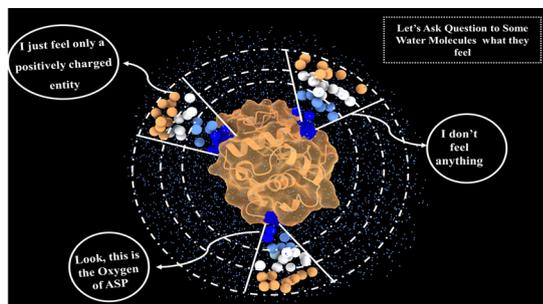
3916

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



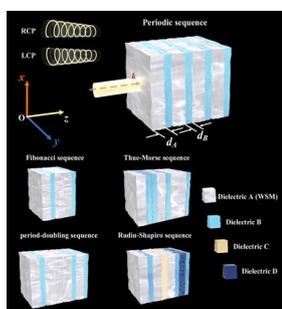
3930



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

Subhabrata Hazra and Biman Jana*

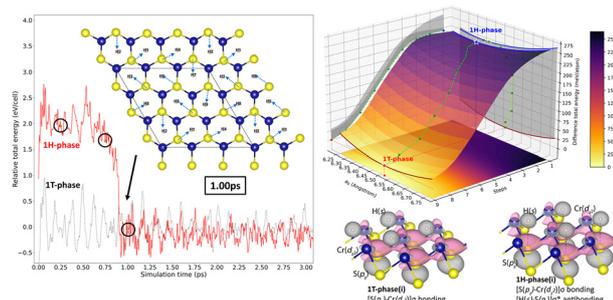
3941



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

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

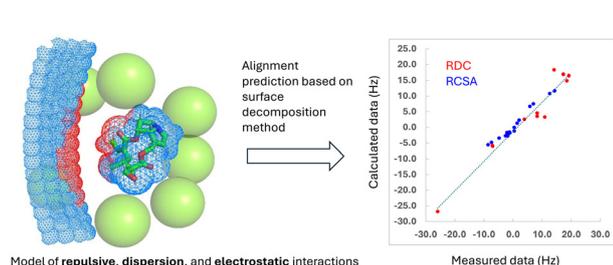
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Half-metallic and ferromagnetic phases in CrSH monolayers using DFT+*U* and BO-MD calculations

Akkarach Sukserm, Jakkapat Seeyangnok and Udomsilp Pinsook*

3960



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

Yizhou Liu

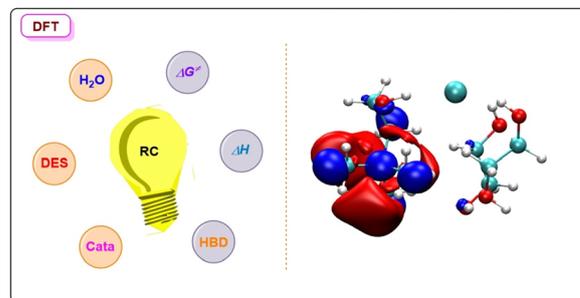


RESEARCH PAPERS

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

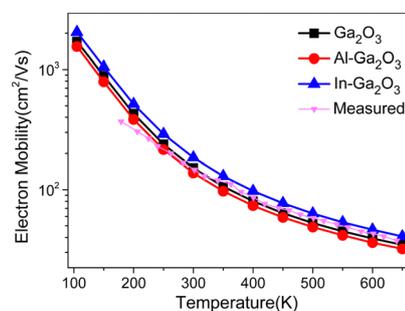
Yan Zhang, Yong Sheng Yang, Shi Jia Zhao, Cui Wei, Ning Zou,* Ying Xue* and Wen Jun Zhou*



3988

First principles investigation of electron mobility enhancement of β -Ga₂O₃ doped with indium

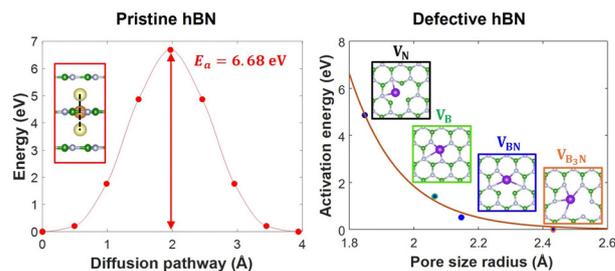
Leng Zhang,* Jiajian Huang, Yuhao Shen, Fei Liu, Pengzhan Zhang, Danbei Wang, Kongping Wu and Yaowei Wei



3997

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*

