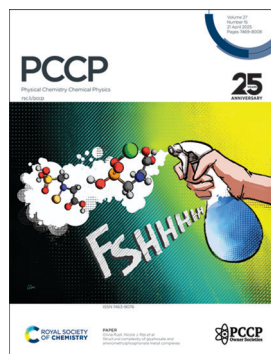


IN THIS ISSUE

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Cover

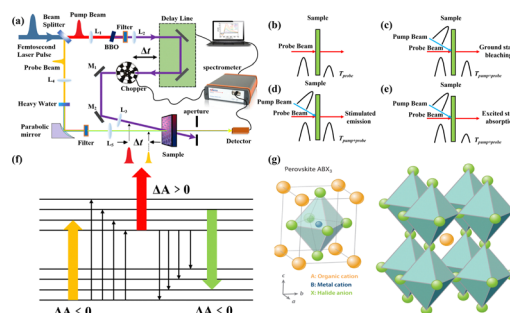
See Olivia Rusli, Nicole J. Rijs *et al.*, pp. 7519–7531. Image reproduced by permission of Clarissa Rusli from *Phys. Chem. Chem. Phys.*, 2025, 27, 7519.

REVIEW

7485

Advances in hot carrier relaxation dynamics of perovskites with ultrafast time-resolved detection

Wanyun Zhang, Haiying Song,* Abbas Zeeshan, Jing Chen and Shibing Liu

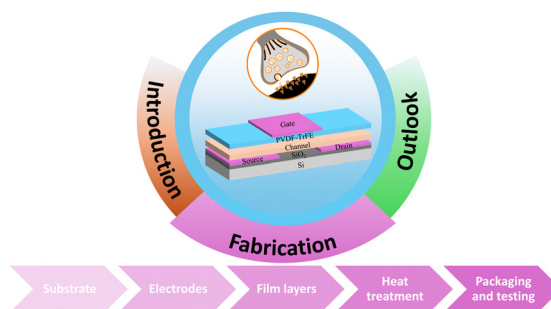


TUTORIAL REVIEW

7502

A review of synaptic devices based on organic ferroelectric materials

Mu Yuan



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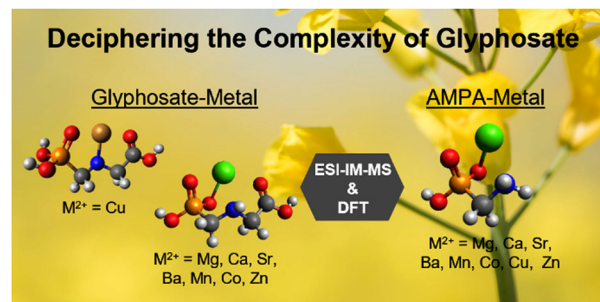
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7519

Structural complexity of glyphosate and aminomethylphosphonate metal complexes

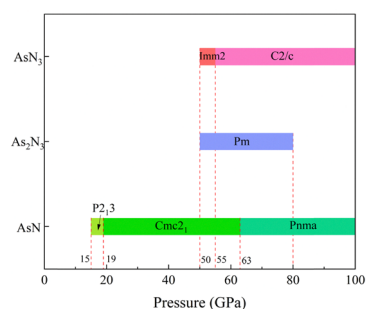
Olivia Rusli, Oscar H. Lloyd Williams, Papri Chakraborty, Marco Neumaier, Frank Hennrich, Sjors Bakels, Kevin Hes, Anouk M. Rijs, Boris Ucur, Shane R. Ellis, River J. Pachulicz, Tara L. Pukala and Nicole J. Rijs*



7532

Exfoliating from high-pressure arsenic–nitrogen compounds: an efficient way to obtain 2D-AsN

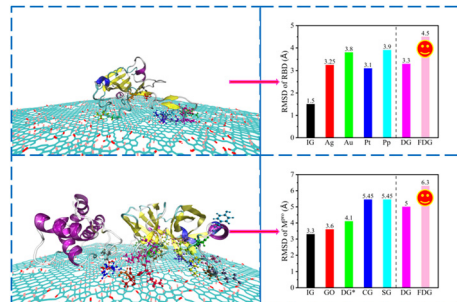
Yanfeng Zhang, Guo Chen, Chengfeng Zhang, Jie Zhang* and Xianlong Wang*



7538

The interface hydrophilic–hydrophobic integration of fluorinated defective graphene towards biomedical applications

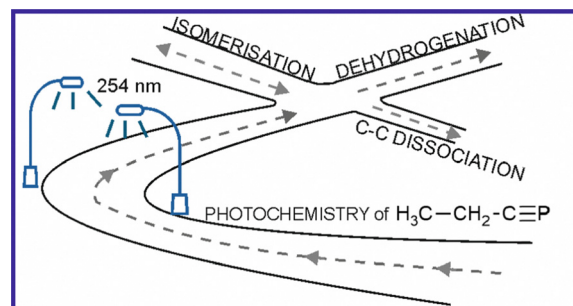
Jiawen Wang, Yi Yu, Huilong Dong, Yujin Ji, Weihua Ning* and Youyong Li*



7556

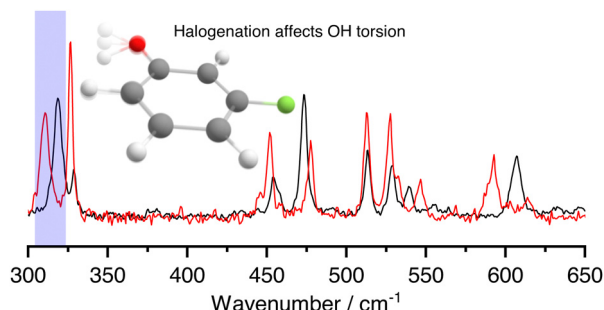
Isomerisation of phosphabutynes and a photochemical route to phosphabutadiyne (HC₃P), a phosphorus analogue of cyanoacetylene

Arun-Libertsen Lawzer,* Elavenil Ganesan, Thomas Custer, Jean-Claude Guillemin and Robert Kotos



RESEARCH PAPERS

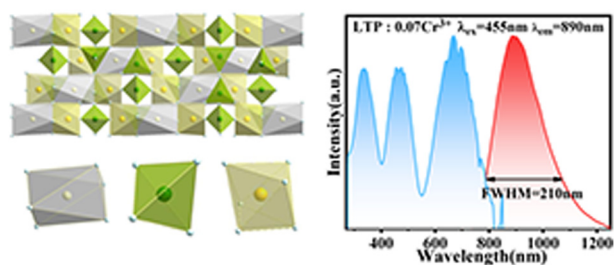
7565



Gas-phase, conformer-specific infrared spectra of 3-chlorophenol and 3-fluorophenol

Olga A. Duda, Gerrit C. Groenenboom, Daniel A. Horke and Joost M. Bakker*

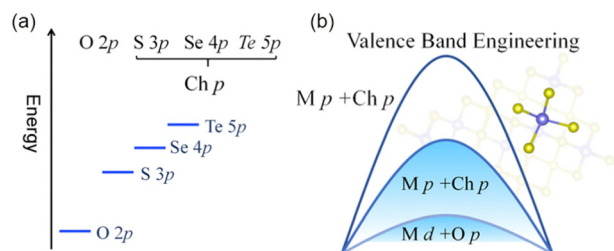
7574



Broadband near-infrared phosphor $\text{LiTi}_2(\text{PO}_4)_3:\text{xCr}^{3+}$ realized via multi-site occupation

Jin Zou, Daoyun Zhu,* Zhongfei Mu,* Song Xu, Nurahmat- Wali, Fugen Wu, Huafeng Dong, Xin Zhang, Yifei Luo and Yuchun Zhan

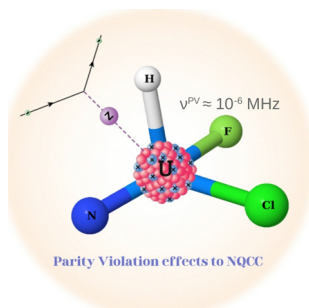
7584



Valence band modulation and the p-type conducting mechanism of LiMCh_2 ($\text{M} = \text{Al, Ga, In}$ and $\text{Ch} = \text{S, Se, Te}$) semiconductors driven by low-electronegativity anions

Mi Zhong,* Zheng-Tang Liu and Qi-Jun Liu

7594



Parity violation effects on the electric field gradient

Juan J. Aucar and Alejandro F. Maldonado*

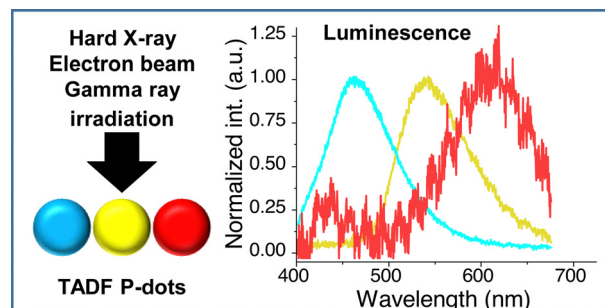


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Color variation in radio-luminescence of P-dots doped with thermally activated delayed fluorescence molecules

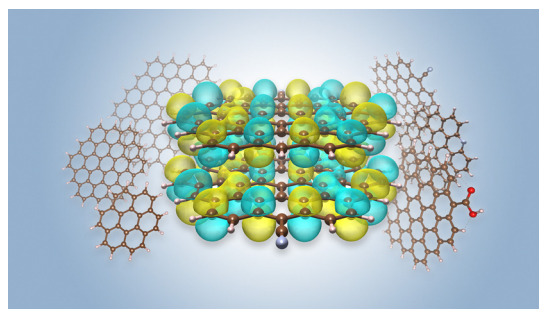
Zheming Su, Hieu Thi Minh Nguyen, Zuoyue Liu, Daiki Asanuma, Minoru Yamaji, Masanori Koshimizu, Hajime Shigemitsu, Sachiko Tojo, Tadashi Mori, Toshiyuki Kida, Guillem Pratx,* Mamoru Fujitsuka* and Yasuko Osakada*



7611

Exploring the electronic properties of carbon nanoflake-based charge transport materials for perovskite solar cells: a computational study

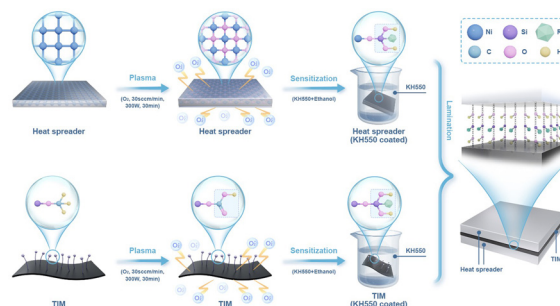
Ruicheng Li, Keisuke Maeda, Keisuke Kameda, Manabu Ihara* and Sergei Manzhos*



7629

Enhanced bonding intensity between the vertically aligned carbon fiber thermal interface material and heat spreader of a flip-chip package through a silane coupling agent

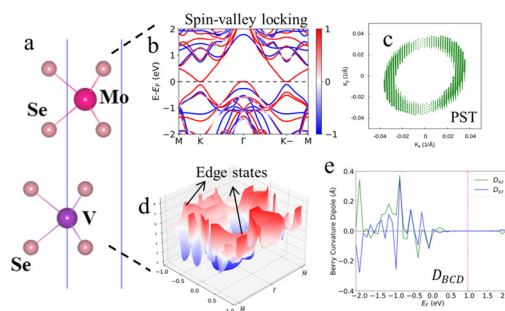
Mingming Yi, Ouwei Liu, Jing Wen, Yiqiu Qiu, Ping Wu, Wenhui Zhu* and Liancheng Wang*



7640

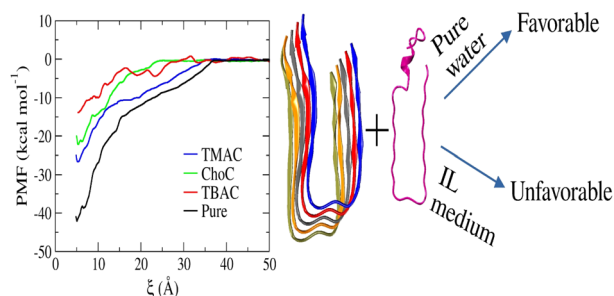
Nonzero Berry curvature dipole, magnetic gapped edge states and persistent spin texture in a rotational symmetry preserved van der Waals magnetic topological insulator

Saransha Mohanty, Anil Kumar Singh, Liyenda Gogoi and Pritam Deb*



RESEARCH PAPERS

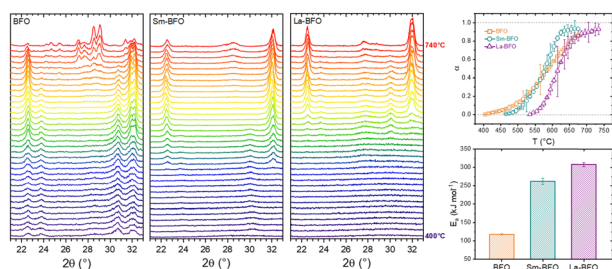
7650



Exploring the structure and stability of pentameric amyloid β peptide aggregates in aqueous ammonium-based ionic liquid solutions

Subhadip Sahoo and Sanjoy Bandyopadhyay*

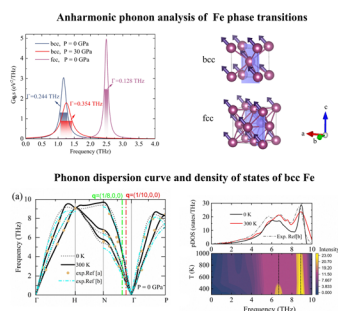
7665



Perovskite phase formation in pure and Sm- and La-substituted BiFeO_3 thin films in isothermal and non-isothermal regimes

M. A. M. Teixeira, F. B. Minussi,* J. A. Eiras and E. B. Araújo

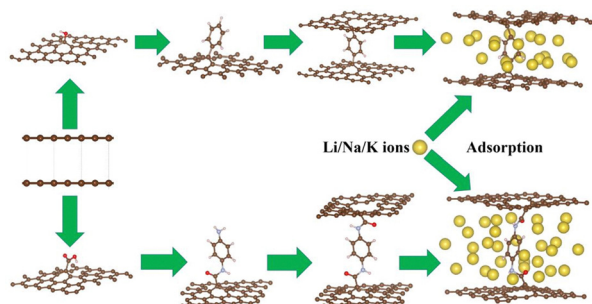
7675



Phase transition of Fe under extreme conditions studied by using an anharmonic phonon approach based on machine learning force fields

Feng-ning Xue, Yong-Chao Wu, Yong Lu* and Jian-Li Shao*

7682



First-principles study on promoting the performance of graphene as an anode material for alkali metal ion batteries by covalent cross-linking of rigid molecules

Zixun Shi, Xiaowei Li,* Kunhe Yi, Chengyang Li, Wenxin Chen and Guocheng Lv*

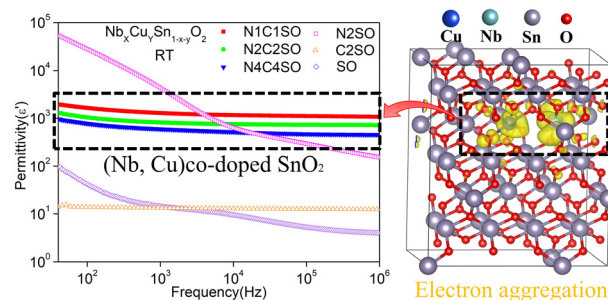


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7692

Electron/hole pinning effects, localization, and dielectric properties in (Nb,Cu) co-doped SnO_2 ceramics

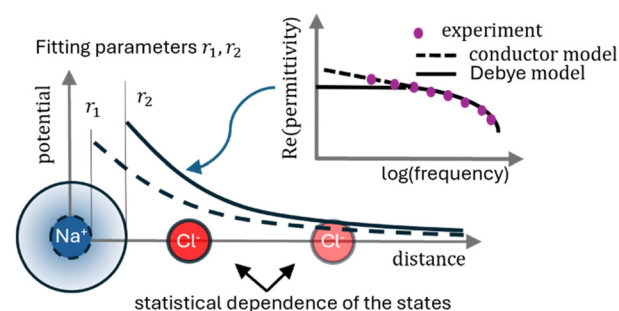
Yu Tan, Yushi Wang, Heng Wang,* Dinghui Xu, Yuanfang Yue, Xiaojun Zheng, Jiafeng Ma, Dandan Gao* and Wanbiao Hu



7703

Fitting ambiguities mask deficiencies of the Debye–Hückel theory: revealing inconsistencies of the Poisson–Boltzmann framework and permittivity

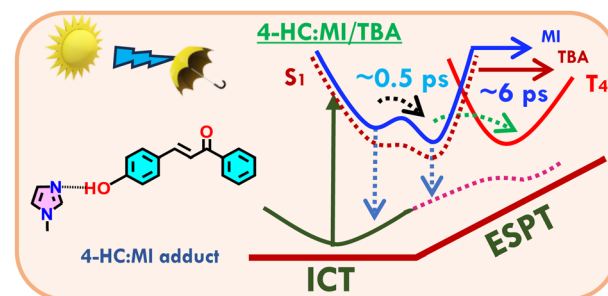
Benjamin Janotta,* Maximilian Schalenbach,* Hermann Tempel and Rüdiger-A. Eichel



7716

Ultrafast excited-state dynamics of 4-hydroxychalcone: role of intramolecular charge transfer and photoacidity

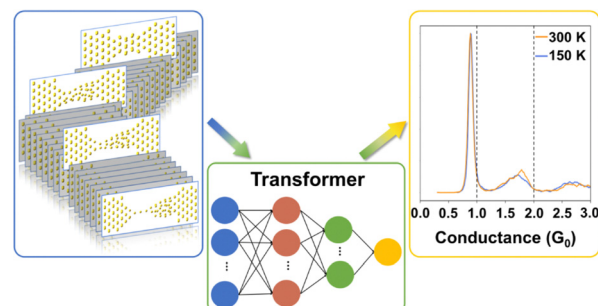
Preetika Verma, Reshma Mathew, Nishant Dhiman, Prajoy Kumar Mitra and Yapamanu Adithya Lakshmana*



7728

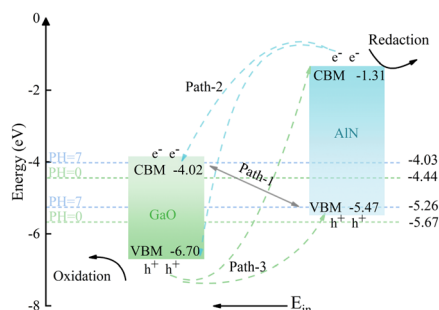
Transformer-based deep learning structure–conductance relationships in gold and silver nanowires

Dongying Lin, Jijie Zou, Yangyu Dong, Yudi Wang,* Yongfeng Wang, Stefano Sanvito and Shimin Hou*



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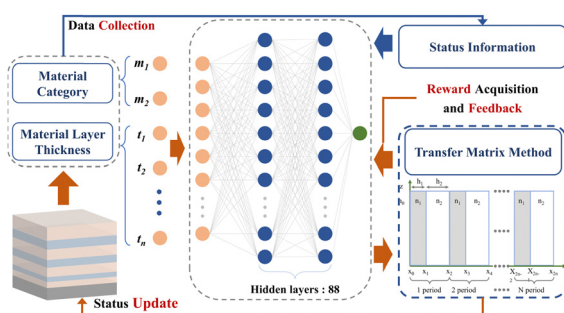
7740



High solar-to-hydrogen efficiency in Z-scheme AlN/GaO heterojunctions for visible light water splitting

Lu Liu, Ning-Ci Zhou, Tong Chen, Cheng Gong,*
Ling-Ling Wang, Kejun Dong and Liang Xu*

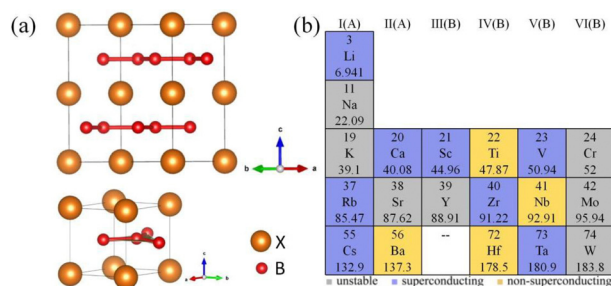
7753



Reinforcement learning-based inverse design of composite films for spacecraft smart thermal control

Yongxing Chen, Haining Ji,* Peng Long, Bin Liu,
Yi Wang, Yangyong Ou, Cong Deng, Yan Huang and
Junlong Wang

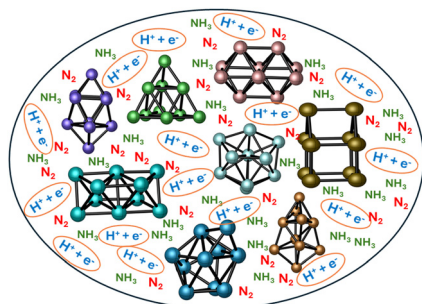
7763



Phonon-mediated superconductivity in the metal diborides XB_2 under pressure

Zhi-Yuan Qiu, Wen-Guang Li,* Zheng-Tang Liu and
Qi-Jun Liu

7773



Electrocatalytic reduction of nitrogen to ammonia on metal nanoclusters: insights and trends from d- and p-block metals

Rajesh Kumar Raju

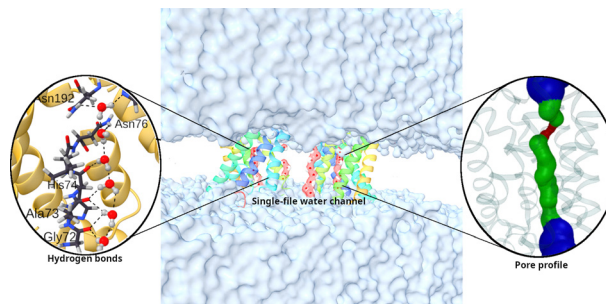


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7797

Analysis of the impact of protein conformational dynamics and intermolecular interactions on water flux through TIP3;1 aquaporins of *Zea mays* L.

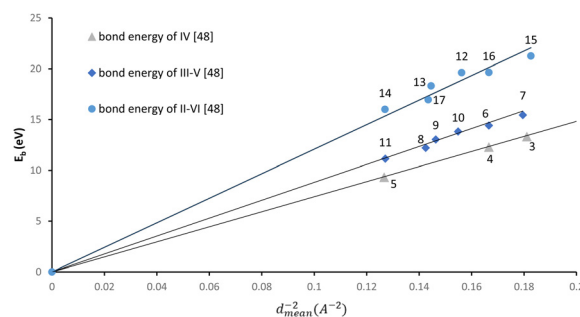
Diego Fernando Nieto-Giraldo,*
 José Mauricio Rodas Rodríguez and
 Javier Ignacio Torres-Osorio



7805

A novel model for bulk modulus and bond energy calculation of Si and its binary compounds, tetrahedral ternary semiconductors in bulk and nanocrystals

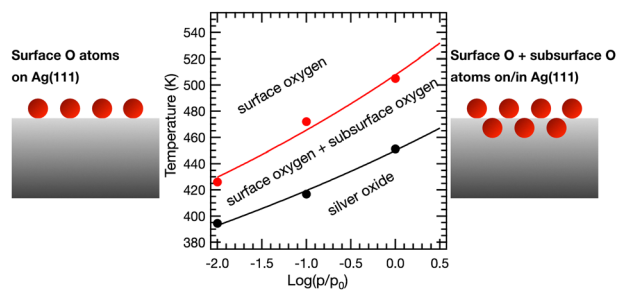
Nzar Luqman Muttalib* and Botan Jawdat Abdullah



7816

Modeling the subsurface adsorption of atomic oxygen in silver from high vacuum to high pressure

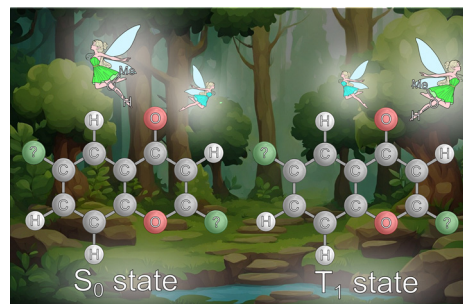
Carson J. Mize, Lonnie D. Crosby, Elizabeth K. Lander
 and Sharani Roy*



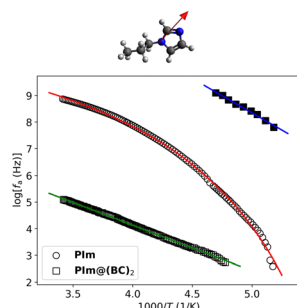
7826

Influence of substitution patterns on isomer preference in 1:1 chromone–methanol complexes

Natalia Moreira Cárcamo, Patrick H. Strebert and
 Fabian Dietrich*



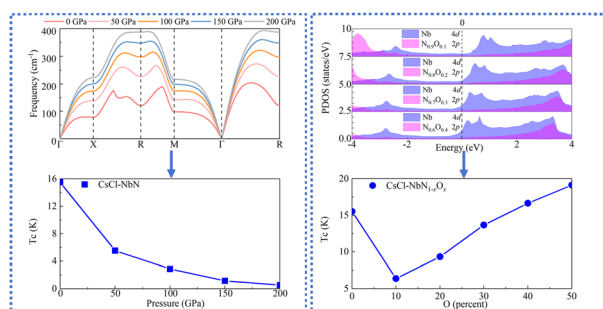
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Guest molecule dynamics and ferroelectric transition in a clathrate compound

Aitor Erkoreka,* Zi-Yi Du, Alberto Oleaga,
Rui-Kang Huang and Josu Martinez-Perdiguerio

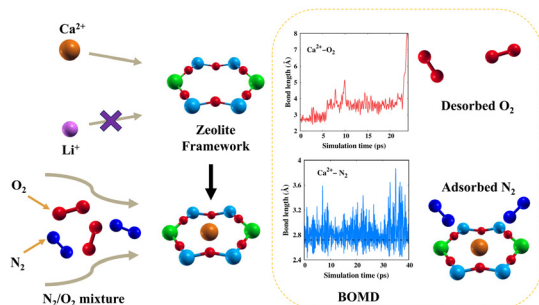
7840



Oxidation-resilient superconductivity in a novel high-hardness superconductor: a first-principles study

Wenhao Fan, Rui Song,* Haiyan Lu* and Cheng Lu*

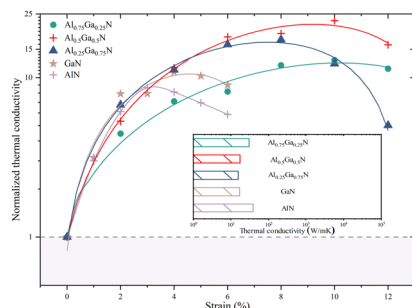
7846



Evaluating the preferential adsorption of N₂ from a binary mixture of N₂/O₂ on extra-framework cations of zeolites: a computational and experimental study

George Devasia, Sachin U. Nandanwar and
Sailaja Krishnamurthy*

7858



Super strain enhanced thermal conductivity of monolayer aluminum/gallium nitride (Al_xGa_{1-x}N) alloys

Xiaoxia Wang, Zhunyun Tang, Linfeng Yu, Donghai Wei,
Qikun Tian, Chao Tang, Hongjun Xiang, Huimin Wang,*
Tao Ouyang* and Guangzhao Qin*

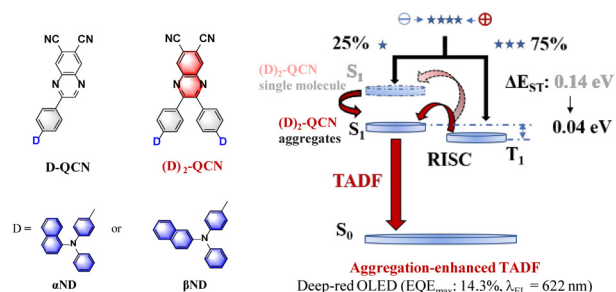


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7866

Aggregation-enhanced TADF in deep-red emitters for high-performance OLEDs

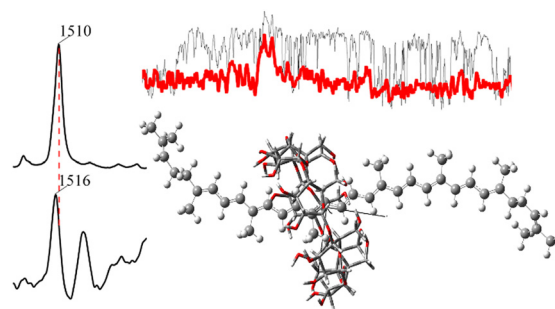
Chengrui Huang, Jianping Zhou, Kerim Samedov, Liang Zhang, Guoqing Peng, Xiangchao Peng, Mingxing Chen, Dongdong Zhang* and Yuanjing Cai*



7874

Interactions of lycopene with β -cyclodextrins: Raman spectroscopy and theoretical investigation

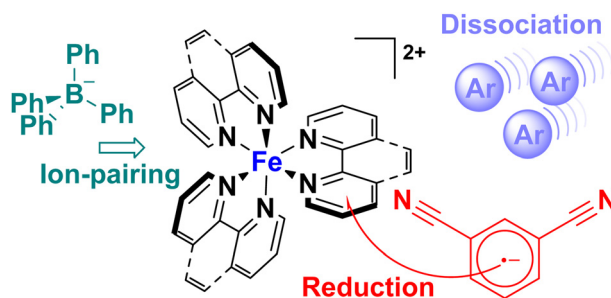
Laurynas Diska, Alma Bockuviene, Rūta Gruskiene, Tatjana Kavleiskaja, Jolanta Sereikaite, Goda Bankovskaite and Mindaugas Macernis*



7882

Evaluating iron diimines: ion-pairing, lability and the reduced state

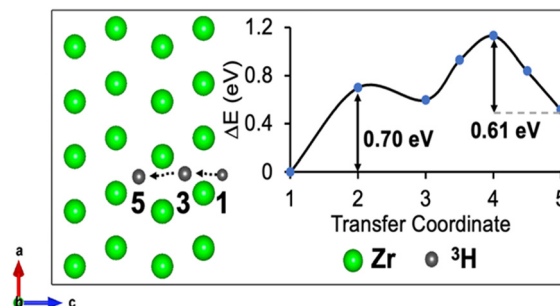
David Schilter,* Umberto Terranova, Caden B. Summers and Rebecca R. Robinson



7893

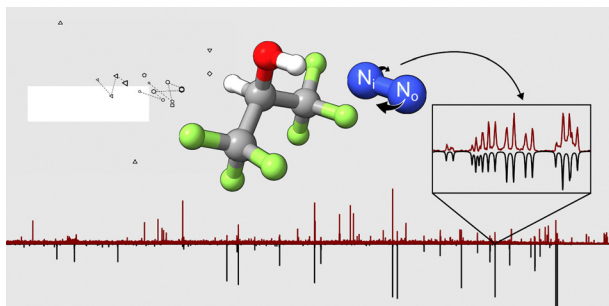
Tritium adsorption and absorption on (100) and (001) surfaces of pure and tin defective zirconium

Morgan Redington, Hari P. Paudel, De Nyago Tafen, Daniel P. Miller, Eva Zurek and Yuhua Duan*



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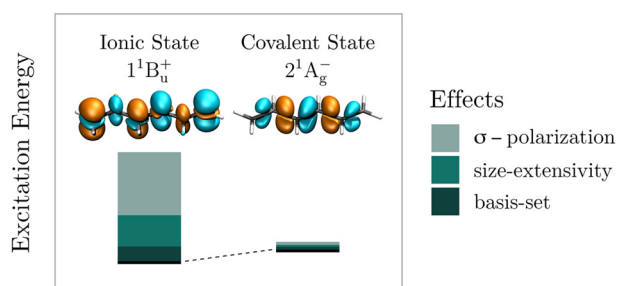
7905



Rotational and vibrational spectroscopy of a weakly bound hexafluoroisopropanol ··· dinitrogen complex: ^{14}N hyperfine splittings, molecular geometry, and experimental benchmarks

Shauna E. Beresnak, Sönke Oswald, Bowei Wu, Nathan A. Seifert, Martin A. Suhm, Wolfgang Jäger and Yunjie Xu*

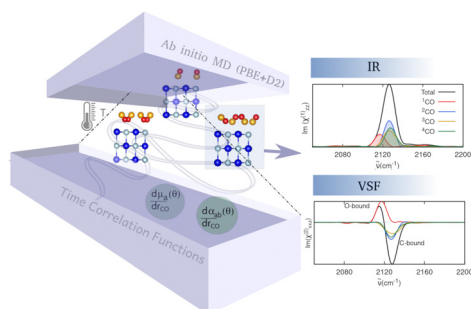
7916



Low-lying excited states of linear all-*trans* polyenes: the σ - π electron correlation and the description of ionic states

Julio C. V. Chagas, Luan G. F. dos Santos, Reed Nieman, Adelia J. A. Aquino, Silmar A. do Monte, Felix Plasser, Péter G. Szalay, Hans Lischka* and Francisco B. C. Machado*

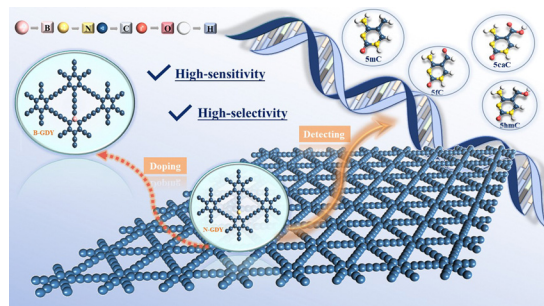
7929



When carbon monoxide goes "upside down": vibrational signatures of CO at NaCl(100) from *ab initio* molecular dynamics

Shreya Sinha,* Alec M. Wodtke and Peter Saalfrank*

7943



B/N modified GDY as a rare base 2D sensor: a first-principles study

Ruiying Zhang, Xia Zeng, Lin Yu, Lingyu Meng, Wenjin Miao and Lingxia Jin*

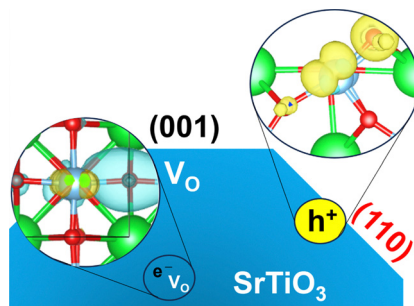


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7954

Facet-dependent polaron stability in photocatalysis by SrTiO₃: a constrained DFT study

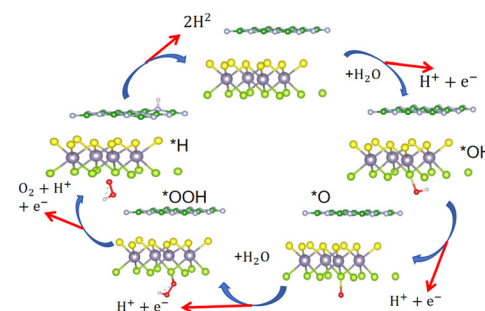
Tatsuya Joutsuka



7965

High performance photocatalytic water splitting in two-dimensional BN/Janus SnSSe heterojunctions: *ab initio* study

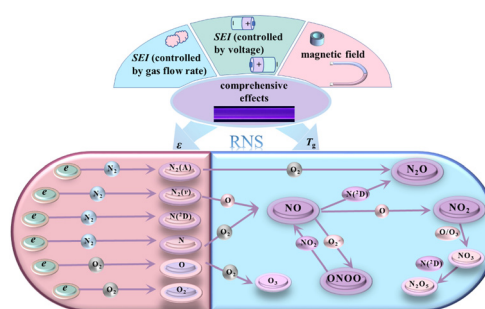
Fan Xiang, RuiHao Tan, QingYu Xie and KaiWang Zhang*



7975

Characteristics of chemical products under the NO_x mode of dielectric barrier discharge: comprehensive effects of specific energy input and magnetic field

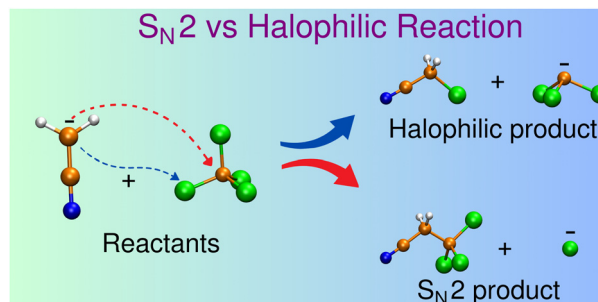
Kun Liu,* Jing Dai and Xiong-Feng Zhou



7987

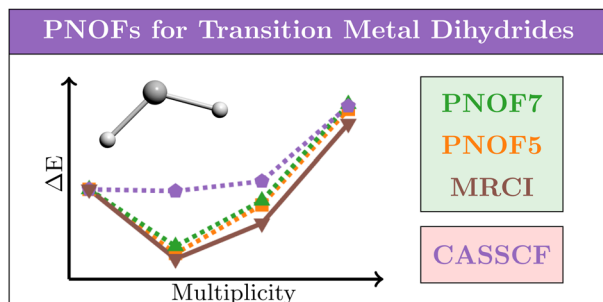
Mechanisms and dynamics of the halophilic reaction between CH₂CN⁻ and CCl₄

Siddharth Sankar Dutta, Sayoni Mitra and Upakarasamy Lourderaj*



RESEARCH PAPERS

7997



Assessment of the Piris natural orbital functionals on transition metal dihydrides

Lizeth Franco, Roberto Rojas-Hernández, Iván A. Bonfil-Rivera, Emilio Orgaz* and Jorge M. del Campo*

CORRECTION

8005

Correction: Isomerisation of phosphabutynes and a photochemical route to phosphabutadiene (HC₃P), a phosphorus analogue of cyanoacetylene

Arun-Libertsen Lawzer,* Elavenil Ganesan, Thomas Custer, Jean-Claude Guillemin and Robert Kotos

