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Cover

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Inside cover

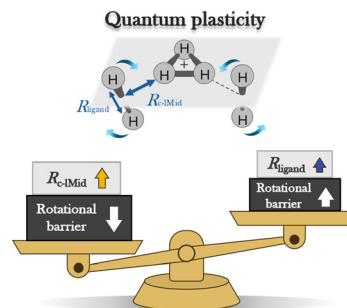
See Jan-Michael Y. Carrillo, V. N. Ravi Kishore Vutukuri et al., pp. 8334–8348. Image reproduced by permission of V. N. Ravi Kishore Vutukuri from *Phys. Chem. Chem. Phys.*, 2026, **28**, 8334. Image created using Google Gemini.

COMMUNICATIONS

8308

Microscopic origin of quantum plasticity in small $H_3^+(H_2)_n$ ($n = 1-3$) clusters revealed by path integral molecular dynamics simulations

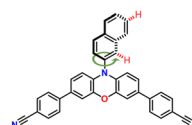
Kotomi Nishikawa, Hikaru Tanaka, Kazuaki Kuwahata, Masanori Tachikawa and Taro Udagawa*



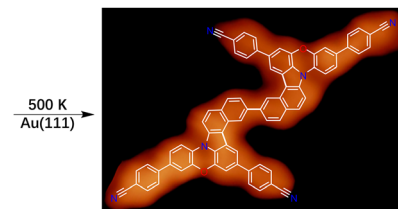
8312

Selective aryl C–H activation governed by molecular nonplanar conformation on Au(111)

Shenwei Chen, Lixia Kang, Haiwei Wang, Xiang Zhang, Tong Xiangli, Suyu Dai, Zhe Huang, Maoyun Lang, Yongjie Chen, Yucheng Song, Cunfeng Zheng, Zechao Yang, Haimin Shen,* Chao Xiong* and Jin Li*



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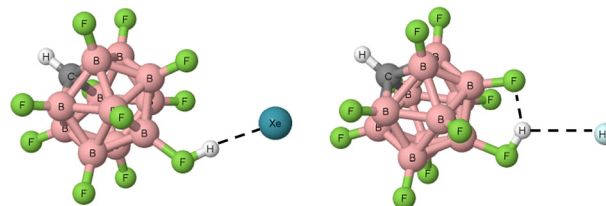
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COMMUNICATIONS

8318

Hydrogen bonds in complexes of noble gases with H(CHB₁₁F₁₁) carborane acid – DFT calculations

Sławomir J. Grabowski

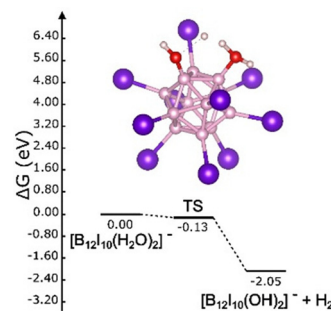


RESEARCH PAPERS

8323

Spontaneous generation of hydrogen from water using modified dodecaborate ions

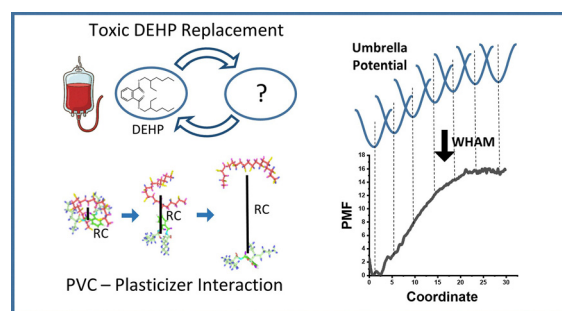
Hugo A. López Peña and Puru Jena*



8334

Investigating PVC polymer–plasticizer interactions with atomistic MD simulations and potential of mean force calculations

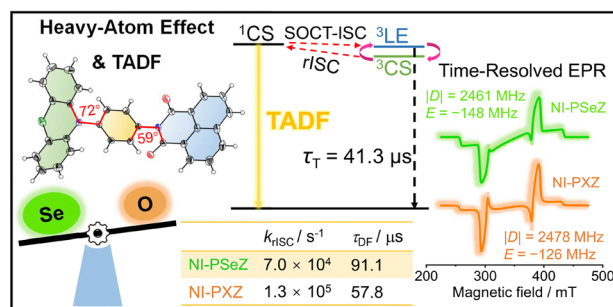
Sai Athmeeya G. Shet, Jan-Michael Y. Carrillo,* Jacek Jakowski, S. S. R. Kumar Challa and V. N. Ravi Kishore Vutukuri*



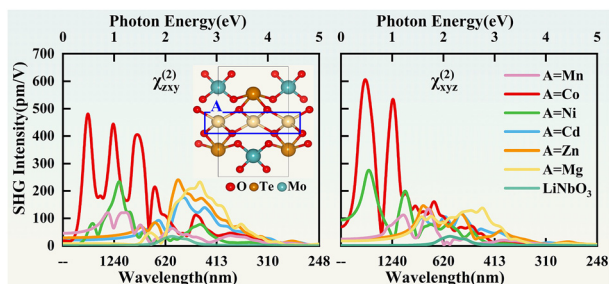
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The effect of heavy atoms on the thermally activated delayed fluorescence properties of naphthalimide–phenoselenazine electron donor–acceptor dyads: electron transfer and intersystem crossing

Peiwen Jiang, Haotian Bai, Yuying Pei, Antonio Toffoletti, Jianzhang Zhao,* Yanqin Li,* Yan Wan* and Antonio Barbon*



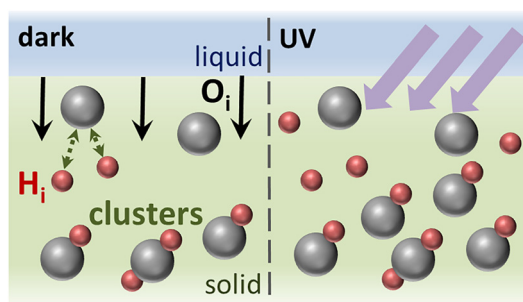
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Regulating second harmonic generation of telluromolybdate materials by atomic substitution

Hongsheng Liu, Qiutong Zhao, Shi Qiu, Luneng Zhao, Anbing Zhang, Fuwen Qin,* Chunyu Ma* and Junfeng Gao

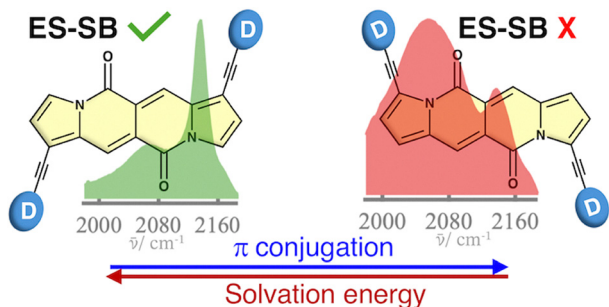
8372



Ultraviolet photoeffects on oxygen–hydrogen interstitial clusters in rutile TiO₂

Heonjae Jeong, Ian I. Suni, Raylin Chen, Grace McKnight, Elif Ertekin, Xiao Su and Edmund G. Seebauer*

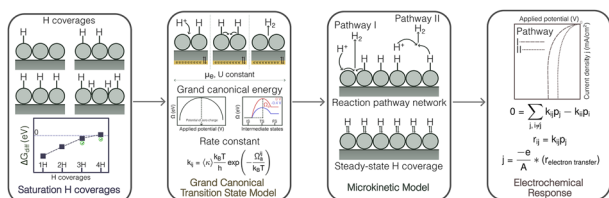
8387



Influence of the substitution pattern on exciton localisation in centrosymmetric quadrupolar dyes

Chinju Govind, Kamil Skonieczny, Daniel T. Gryko* and Eric Vauthey*

8396



Electrochemical hydrogen evolution on Ni₂P: insights from constant-potential DFT and microkinetic modelling

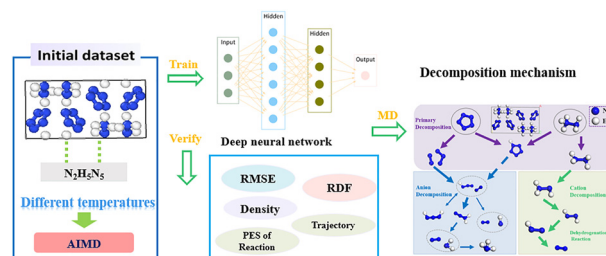
Syam Sadan, Sander Øglænd Hanslin, Ingeborg-Helene Svenum and Jaakko Akola*



8408

The thermal decomposition mechanism of energetic cyclopentazolate salt $N_2H_5N_5$: a deep neural network potential accelerated molecular dynamics study

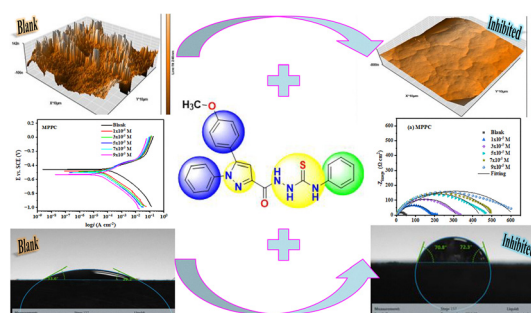
Jiao Zhang, Caimu Wang, Renyi Li, Danyang Zhang, Yaozhong Liu, Guozhen Sheng and Wei Guo*



8419

Robust pyrazole-based thiourea scaffolds as carbon steel corrosion inhibitors in 1 M HCl, complemented by electrochemical and theoretical approaches

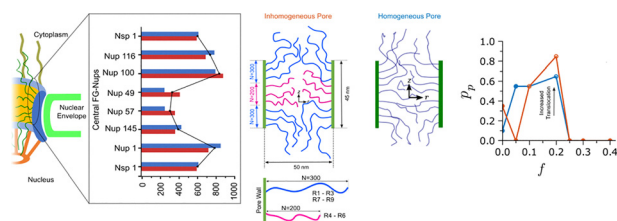
Amira W. Elherbity, Eslam A. Ghaith, A. S. Fouda and Ahmed Fathi Salem Molouk*



8442

FG-Nup sequence length polydispersity enhances selectivity of nuclear pore complex translocation

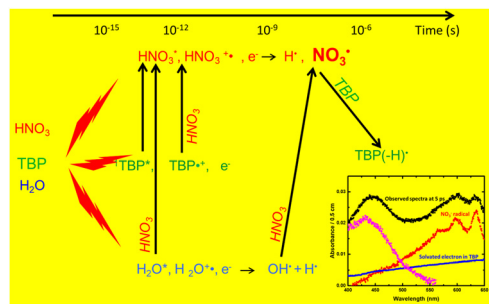
Manoj K. Patel, Lokesh Soni and Ajay S. Panwar*



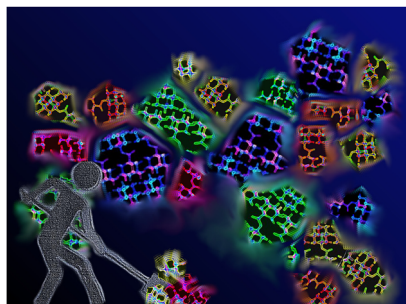
8458

Picosecond time-resolved investigation of NO_3^{\bullet} in PUREX solvent

Amel Zorai,* Daniel Adjei, Mireille Benoît, Sergey Denisov, Philippe Moisy, Jacqueline Belloni and Mehran Mostafavi*



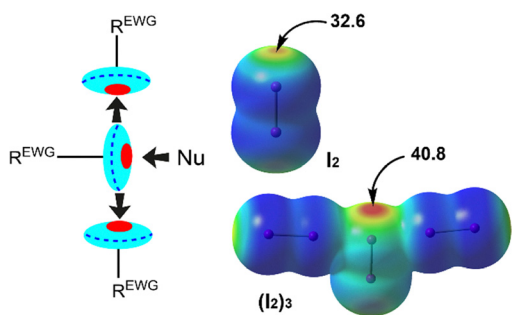
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Self-assembly of structurally rigid diamondoid esters on a HOPG surface

Nataša Burić, Cosme González Ayani, Tomislav Vuletić, Margareta Sohora, Zoran Štefanić, Ida Delač* and Marina Šekutor*

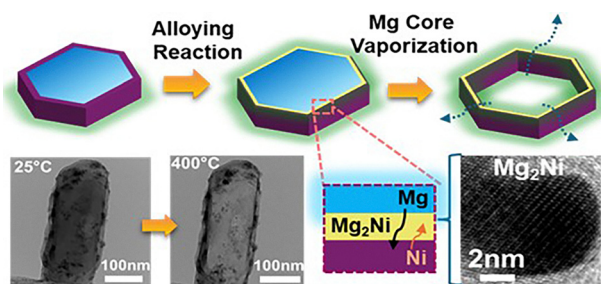
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Noncovalent chemical chameleons in action: positive cooperativity of trifurcated halogen bonds in $2I \cdots I \cdots Nu$ assemblies

Nadezhda A. Bokach, Vadim Yu. Kukushkin, Rosa M. Gomila and Antonio Frontera*

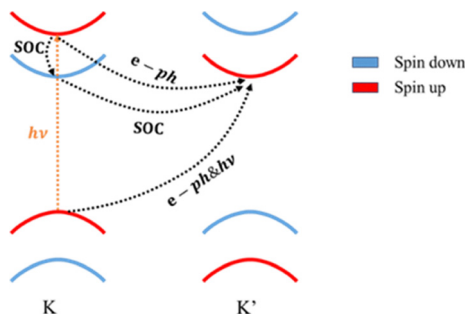
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Intermetallic reaction and eutectic transitions tune the reactivity in core-shell Mg/Ni nanoparticles

Mahbub Chowdhury, Lei Yang, Brandon Wagner, Yuxin Zhou, Lorenzo Mangolini* and Michael R. Zachariah*

8496



Spin valley dynamics of phonons entangled with circularly polarized light in WSe_2

Guodong Liu, Chundan Lin,* Sen Wang, Meiqi Si, Changjin Shao* and Zhenqing Yang*

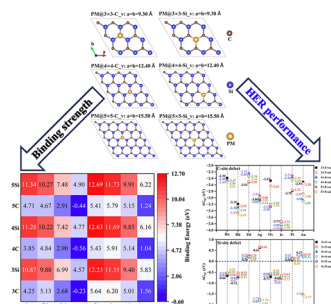


RESEARCH PAPERS

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Modulating the electronic properties and hydrogen evolution reaction performance of precious-metal on 2D-SiC via surface defects

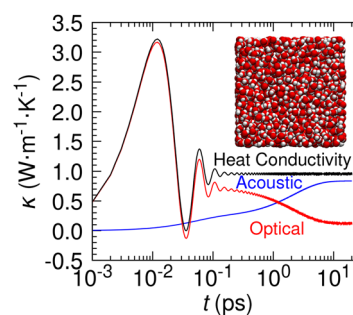
Wenzhong Li,* Xiefei Song and Yuqiong Shan



8514

Molecular simulations of the thermal conductivity of liquid water using the TIP4P/Ice and TIP4P/2005 models

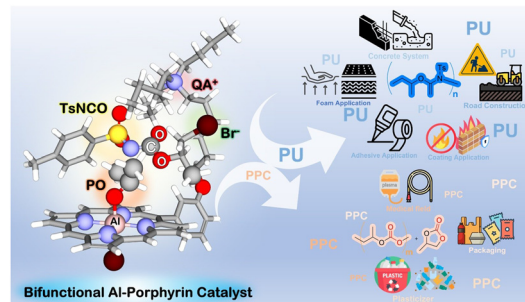
Dongliang Jin



8522

DFT-based mechanistic study of a bifunctional Al-porphyrin catalyst for CO₂/PO and TsNCO polymerizations toward polycarbonates and polyurethanes

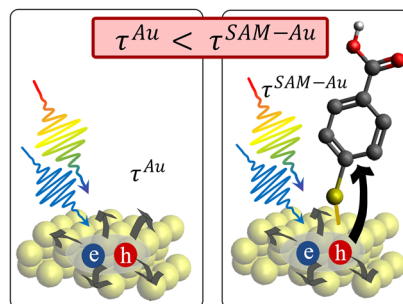
Manussada Ratanasak, Yuwanda Injongkol* and Yasuteru Shigeta*



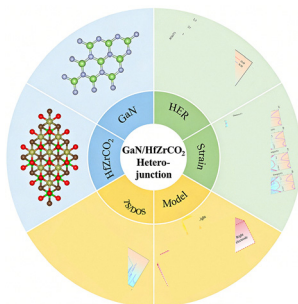
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Phonon-mediated ultrafast dynamics in self-assembled monolayers of 4-mercaptobenzoic acid on gold

Savini Bandaranayake, Paul Schrader, Guangzhao Chen, Liang Z. Tan, Mohana Shivanna, Vitalie Stavila, Juan R. Luna and Krupa Ramasesha*



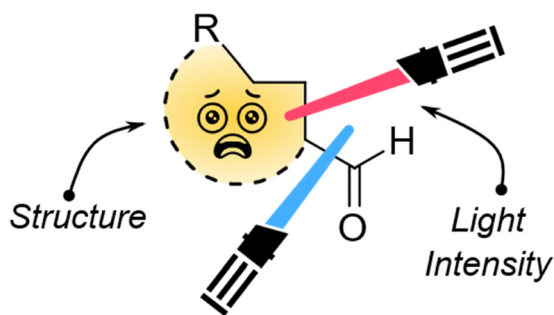
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A GaN/HfZrCO₂ heterojunction with excellent photoresponse and superior hydrogen evolution reaction performance

Zhuo Diao, Zhen Cui* and Shuang Zhang*

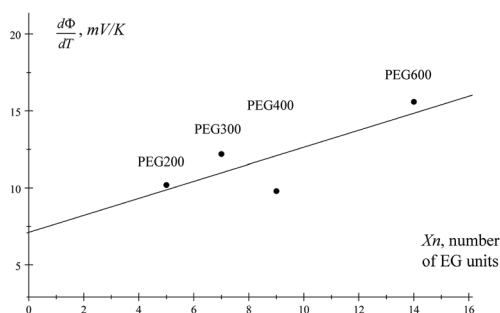
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Disentangling Norrish-type and Rh catalysed decomposition of aldehydes for use as CO donors

Jasmin Hack, Alina Schmitt, Maik Seemann, Daniel Pech, Tianbai Huang and Robert Geitner*

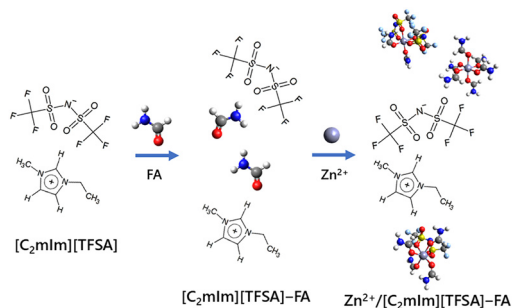
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Seebeck effect in ternary ionic liquids

Semen N. Semenov* and Martin E. Schimpf

8573



Effects of hydrogen-bonding properties of formamide on complex formation with zinc(II) ions in ionic liquid [C₂mIm][TFSA]

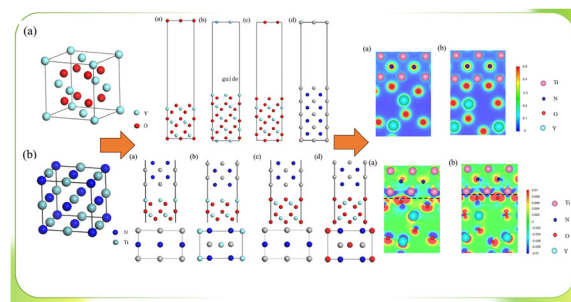
Mikio Maseda and Toshiyuki Takamuku*



8587

Prediction of the interfacial relationship between Y_2O_3 and TiN using first-principles calculations

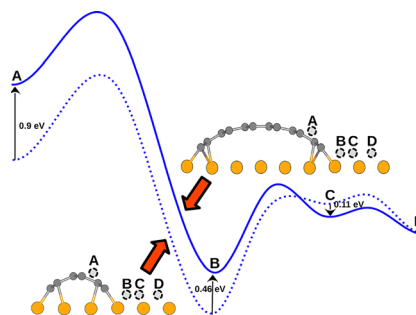
Xiao Yun, Xuejun Ren,* Huixin Zheng, Sha Liu,*
Yefei Zhou, Jing Guo and Qingxiang Yang*



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Edge-driven adatom kinetics in graphene nanoribbon growth on Cu(111)

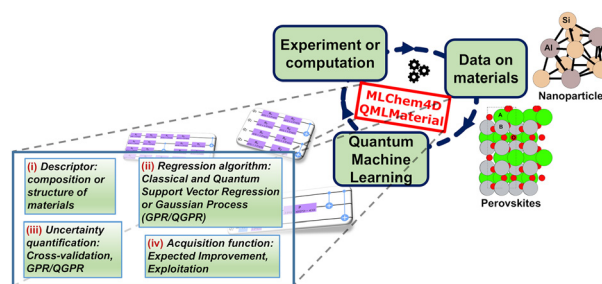
Alexandr Alexeev* and Sergey N. Filimonov



8604

Exploring quantum active learning for materials design and discovery

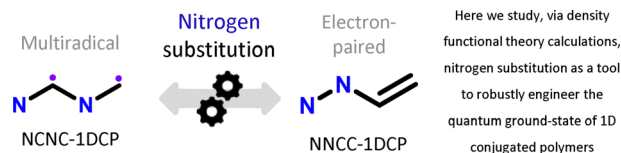
Maicon Pierre Lourenço,* Hadi Zadeh-Haghighi,
Jiří Hostaš, Mosayeb Naseri, Daya Gaur, Christoph Simon
and Dennis R. Salahub



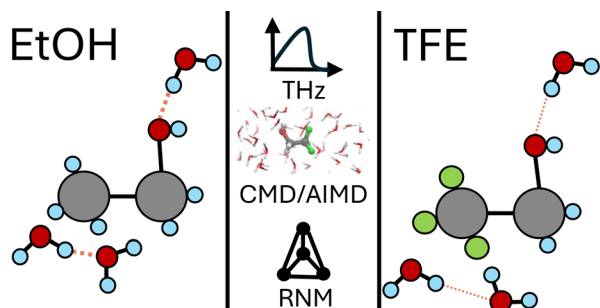
8618

Quantum engineering of mixed-valence 1D conjugated polymers

Lesly Katherine Sánchez De La Cruz, Jordi Ribas-Arino,
Stefan T. Bromley and Isaac Alcón*



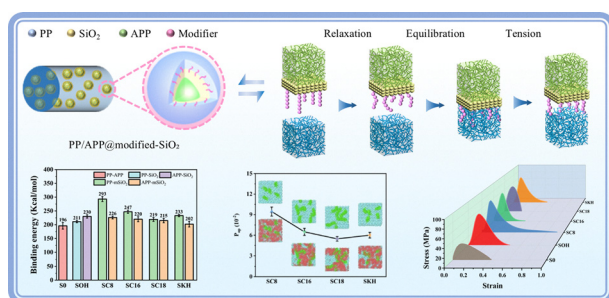
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Perfluorinated alkyl groups induce unexpected hydrophobic hydration structure

Simon Schulke, Elio Casalini, Jaspreet Kaur, Sulejman Skoko, Gerhard Schwaab, Martina Havenith* and Ana Vila Verde*

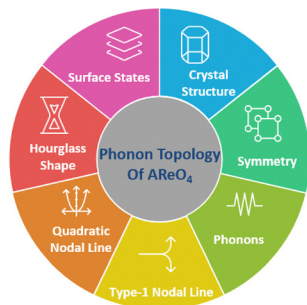
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Effects of modified silica on the interfacial behaviour of polypropylene/ammonium polyphosphate composites: a molecular dynamics study

Xinran Dai, Yueying Sun, Shuai Li, Yanchen Li, Xiaolong Tang, Chunsheng Li* and Jitao Liu*

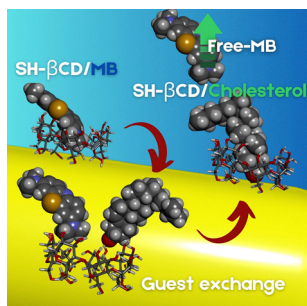
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Investigation of topological nodal line phonons in rhenium-based alkali metal oxides ($A\text{ReO}_4$; $A = \text{Na}, \text{K}, \text{ and Rb}$) using first principles methods

Sathani Maddileti, Aiswarya T, Alfonso Muñoz, Daniel Errandonea, Brendan J. Kennedy and G. Vaitheeswaran*

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Cholesterol-driven guest exchange tunes plasmon damping in single β -cyclodextrin-modified gold nanorods

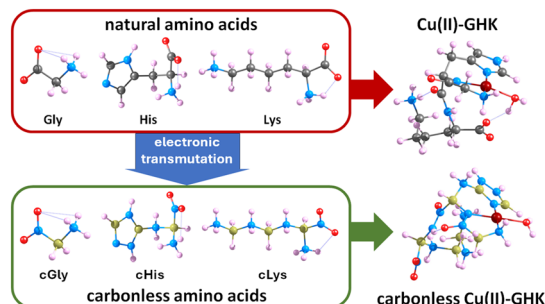
Na Hyun Kim, Metya Indah Firmanti and Ji Won Ha*



8675

Carbonless amino acids and a carbonless GHK peptide

Piotr Skurski* and Iwona Anusiewicz

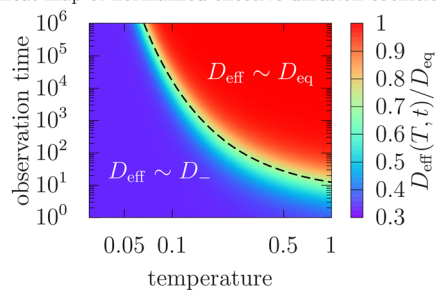


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Observation-time-induced crossover from fluctuating diffusivity

Masahiro Shirataki and Takuma Akimoto*

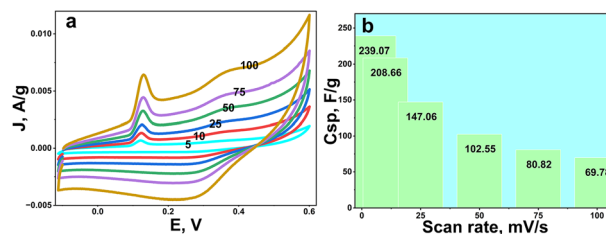
Heat map of normalized effective diffusion coefficient



8706

Bioinspired silver nanoparticles from *Artemisia lerchiana* as durable electrodes for next-generation supercapacitors

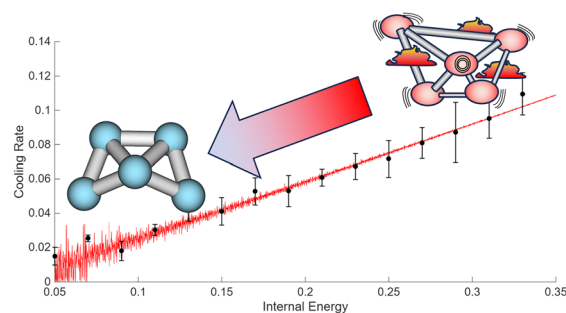
Gunay Hasanova, Sabina Omarova, Nailya Abdullayeva, Rovshan Khalilov, Afat Mammadova, Mehmet Firat Baran,* Abdulkadir Levent,* Mehmet Tevfik Adican, Aziz Eftekhari, Taras Kavetsky,* Ondrej Šauša, Evgeny Katz* and Oleh Smutok



8715

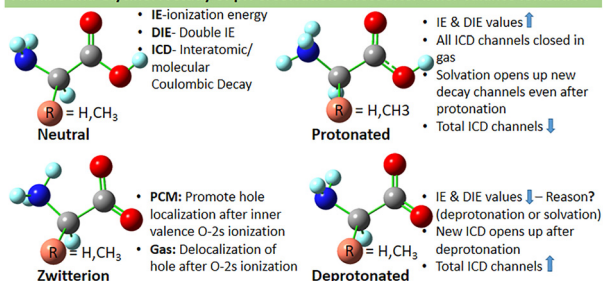
Radiative cooling of isolated Al_5^- cluster ions observed on ultralong timescales as a test case for the validity of the harmonic cascade model

Yehuda Ben Shabo, Damian Müll, Viviane C. Schmidt, Klaus Blaum, Paul Fischer, Sebastian George, Manfred Grieser, Florian Grussie, Oded Heber, Mark A. Iron, Oldřich Novotný, Lutz Schweikhard, Andreas Wolf, Daniel Zajfman, Aigars Znotins, Holger Kreckel* and Yoni Tokor



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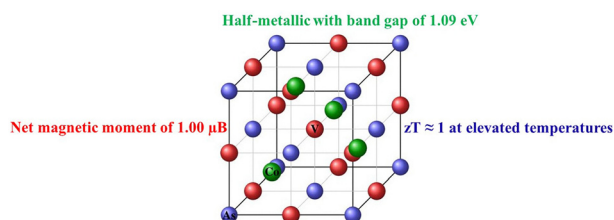
Alanine and Glycine: A study of pH & solvation effect after inner valence ionization



Solvent and pH effects on the ionization energies of bio-organic molecules: a case study of alanine and glycine

Ravi Kumar,* Aryya Ghosh and Nayana Vaval*

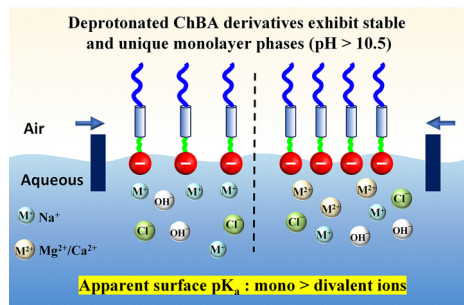
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Unveiling the potential of cobalt-based half-Heusler alloys for multifunctional advanced technological applications: insights from DFT

Sumit Kumar, Diwaker, Arvind Sharma, Karan Singh Vinayak and Shyam Lal Gupta*

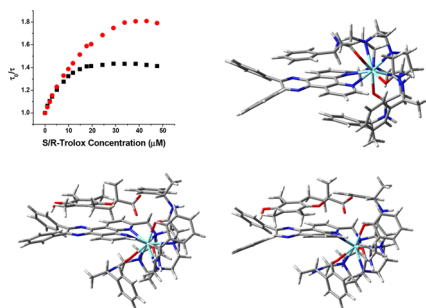
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Influence of pH and salt on the ionization state and phase behavior of some aromatic acid derivatives of cholesterol at the air-aqueous interface

V. M. T. Naidu Moram, Santosh Y. Khatavi, Channabasaveshwar V. Yelamaggad and Padmanabhan Viswanath*

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Dynamic chiral quenching of europium and terbium excited states

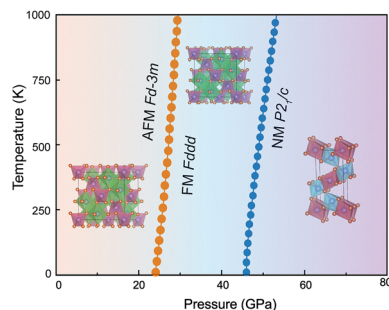
Xinyi Wen, Dominic J. Black, Mark A. Fox, Robert Pal and David Parker*



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Pressure-induced phase transitions in Co_3O_4 : a first-principles study

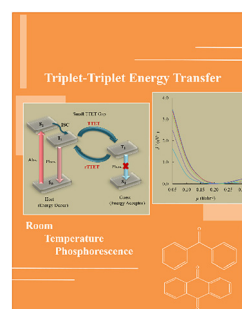
Yaping Xie, Ming Li* and Cong Li*



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Room temperature phosphorescence based on triplet–triplet energy transfer in host–guest systems: excited-state alignment and rational design using range-separated hybrids

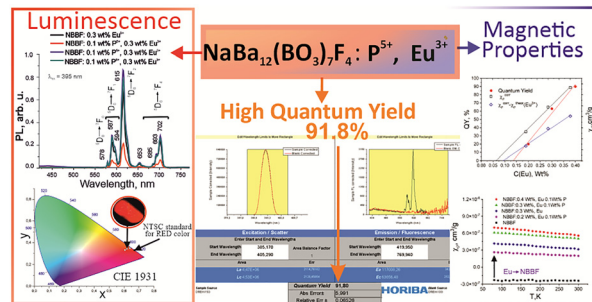
Fatemeh Vaziri Alamdarloo and Mojtaba Alipour*



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High quantum yield luminescence and magnetic properties of $\text{NaBa}_{12}(\text{BO}_3)_7\text{F}_4$ phosphors

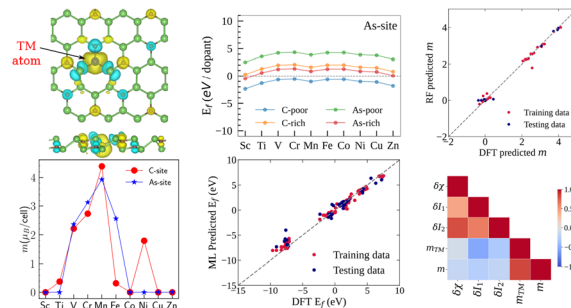
Evgeniy V. Korotaev,* Tatyana B. Bekker, Alexey A. Ryadun, Alexey V. Davydov and Elena B. Baykalova



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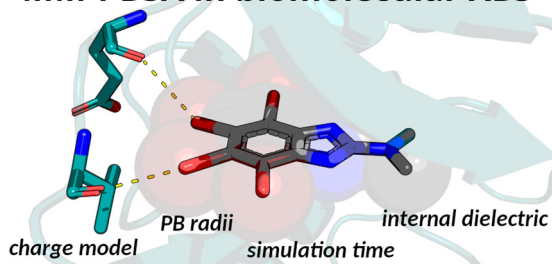
Energetic, geometric, electronic and magnetic properties of transition-metal-substituted binary CA_3 Dirac monolayers

Amrendra Kumar, Muthu Vallinayagam, G. Tejaswini, Anjana E. Sudheer, Rajeev Dutt, Matthias Zschornak, D. Murali and C. Kamal*



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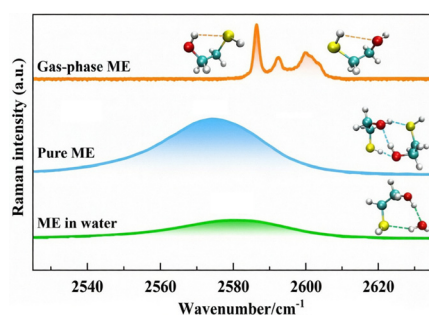
MM-PBSA in biomolecular XBs



Impact of the halogen PB radii in the estimation of protein–ligand binding energies using MM-PBSA calculations

Andreia Fortuna and Paulo J. Costa*

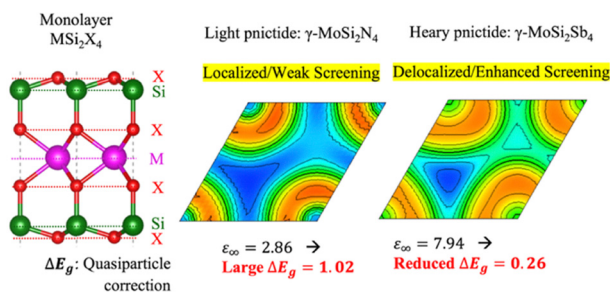
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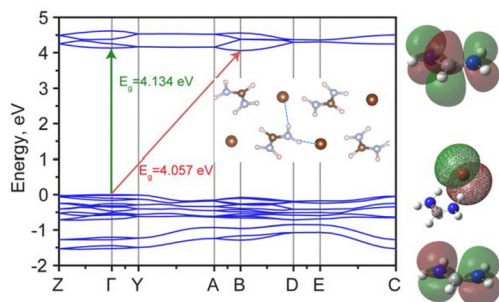
Probing sulfur-centered intra- and intermolecular interactions in mercaptoethanol from the gas to liquid phase: a raman spectroscopic and theoretical study

Siyao Li, Yuhui Li, Xinlang Yang, Yuanqin Yu,*
Xiaoguo Zhou, Rui Zhang, Jinsong Li and Shilin Liu*

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Tailoring the many-body effects and phase configurations in monolayer MSi₂X₄ (M = Mo, W; X = N, P, As, Sb) for wide-range bandgap engineeringYa Yang, Xin Wang, Li Sun, Fanhao Jia, Yurong Ruan,*
Tao Feng* and Yabei Wu*

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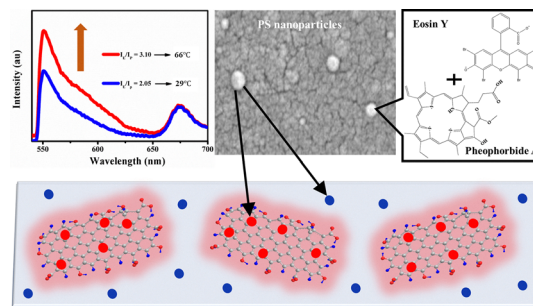
Structure and vibrational spectra of formamidinium bromide

Semyon Zamolotskikh,* Mikhail Smirnov, Dmitrii Pankin
and Evgenii Roginskii

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Polymeric nano-thermometer exploiting reverse intersystem crossing: a potential solution to common interferences

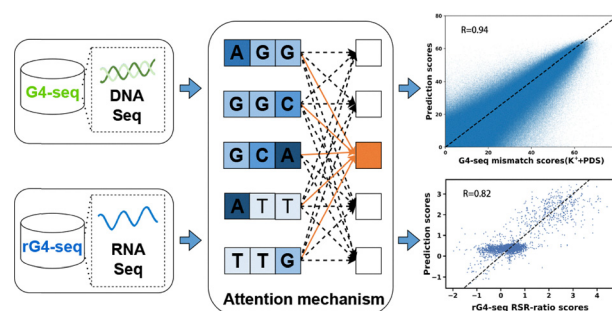
Anwesa Banerjee, Akash Kumar Parida, Anirban Panda, Dibyendu Mallick and Ujjal Bhattacharjee*



8889

TransG4: an interpretable deep-learning approach for sequence-based G-quadruplex prediction

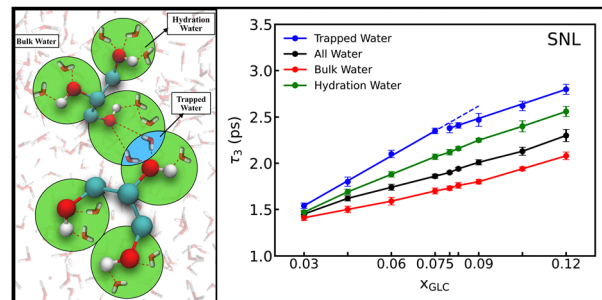
Yongna Yuan,* Yaojie Tian, Zhenyu Liu and Jun Ma



8902

Spectral diffusion in glycerol–water mixtures from theoretical two dimensional infrared spectroscopy: varying effects of concentration for different solvation environments

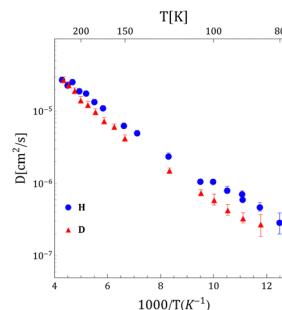
Akshay Kaushik, Ravi Malik and Amalendu Chandra*



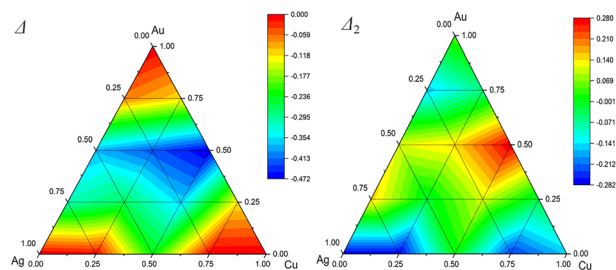
8916

The characteristic function method in surface diffusion

E. E. Torres-Miyares* and S. Miret-Artés



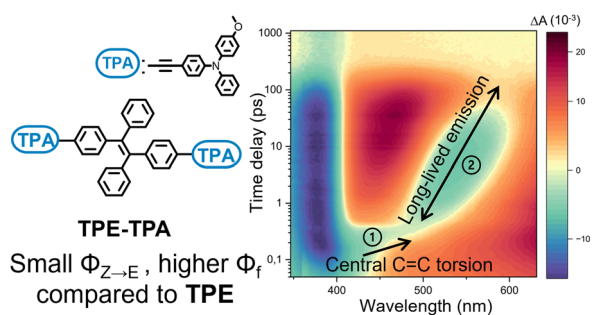
8922



Structural, electronic, optical, and photovoltaic properties of 4-atom Au–Ag–Cu clusters: a first-principles study

Weiyin Li* and Longcan Cheng

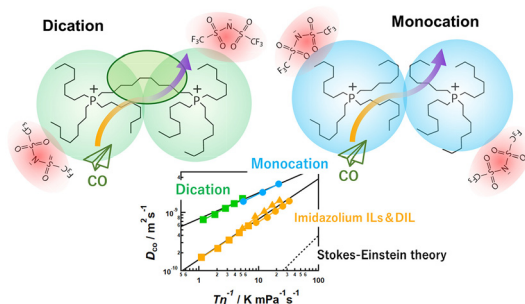
8937



Excited-state dynamics and photochromism of extended tetraphenylethylene derivatives and their control by amino conjugation effect

Mathilde Seinfeld,* Xingjie Fu, Tangui le Bahers,* Chantal Andraud, Stefan Haacke,* Jean Rouillon* and Cyrille Monnereau*

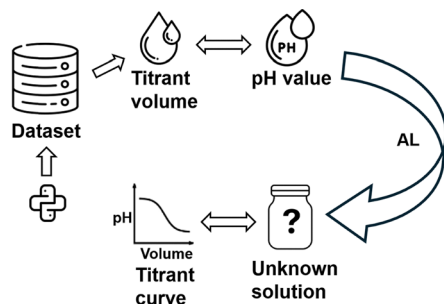
8949



Study on translational diffusion of solute molecules in novel phosphonium-based dicationic ionic liquids by transient grating spectroscopy

Masaki Fujiwara, Shinya Okazoe, Sawaya Suzuki, Koji Osawa, Takatsugu Endo and Yoshifumi Kimura*

8958



A low-cost automated platform for fast and accurate pH control via physics-informed active learning

Quan Yang, Zhipeng Xiang, Zhiwen Zhu, Tairan Yang and Qiang Sun*

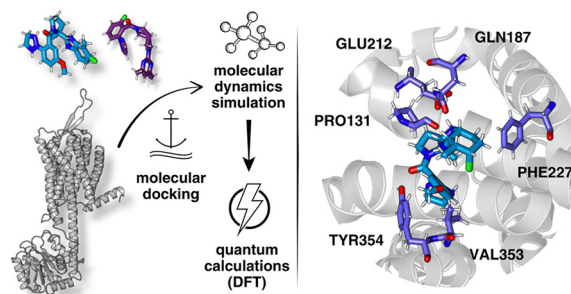


RESEARCH PAPERS

8965

Unveiling the binding mechanism of orexin 2 receptor antagonists with computational chemistry

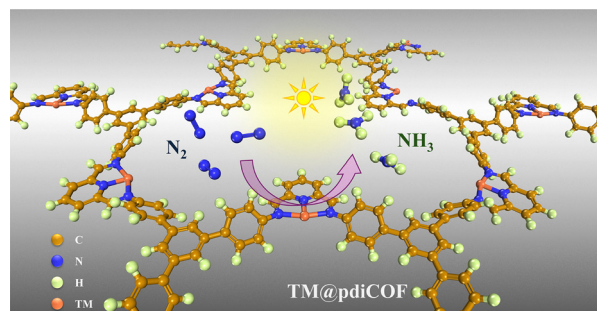
Caio Patricio de Souza Sena,*
 Pedro Corso de Albuquerque, Umberto Laino Fulco,
 Jonas Ivan Nobre de Oliveira and Davi Serradella Vieira*



8981

Coordination engineering in single-atom covalent organic framework photocatalysts for solar-driven nitrogen fixation

Weiguo Li, Helong Wu, Liangchun Wu, Yuan Hu,
 Yuansong Ye, Diwen Liu, Dejing Li, Yanjie Zhang,
 Zuju Ma and Rongjian Sa*



COMMENT

8992

Comment on "Trifluoroacetic acid formation from HFC-134a under atmospheric conditions" by A. Vincent, K. Fujioka, Y. Luo, R. I. Kaiser and R. Sun, *Phys. Chem. Chem. Phys.*, 2026, 28, 4433

Timothy J. Wallington,* John R. Barker, Mads P. Sulbaek Andersen and Ole J. Nielsen

