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Cover

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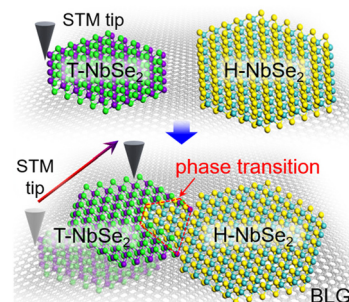
See Harald Agelii, Erik G. Marklund, Carl Coleman *et al.*, pp. 10939–10948. Image reproduced by permission of Erik G. Marklund from *Phys. Chem. Chem. Phys.*, 2025, 27, 10939.

COMMUNICATIONS

10915

Nanoscale island manipulation and construction of heterojunctions by mechanical collision of 2D materials

Xiongbai Cao, Lianguang Jia, Huixia Yang, Zhenru Zhou, Tingting Wang, Haolong Fan, Yan Li, Xiaoyu Hao, Lingtao Zhan, Qinze Yu, Liwei Liu, Teng Zhang, Quanzhen Zhang* and Yeliang Wang*



10923

Noble gas decorated planar tetracoordinate oxygen

Kangkan Sarmah, Farnaz Yashmin, Amit Das, Li-Xia Bai, Jin-Chang Guo* and Ankur K. Guha*



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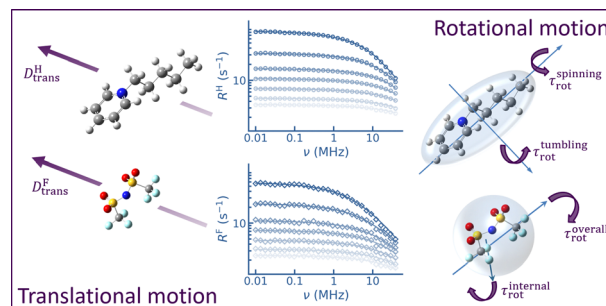


RESEARCH PAPERS

10927

Beyond isotropic reorientation: probing anisotropic and internal motions in ionic liquids with fast field cycling NMR relaxometry and MD simulations

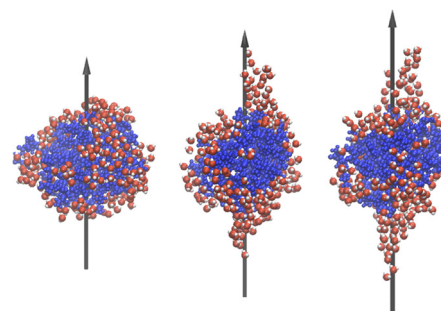
Lennart Kruse, Tanja van Alphen, Johanna Busch, Dietmar Paschek, Ralf Ludwig and Anne Strate*



10939

Dipole orientation of hydrated gas phase proteins

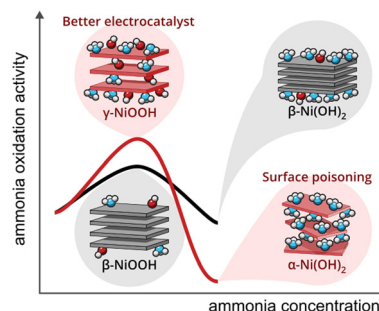
Harald Agelii*, Ellen L. S. Jakobsson, Emiliano De Santis, Gideon Elfrink, Thomas Mandl, Erik G. Marklund* and Carl Coleman*



10949

Ammonia electro-oxidation on nickel hydroxide: phases, pH and poisoning

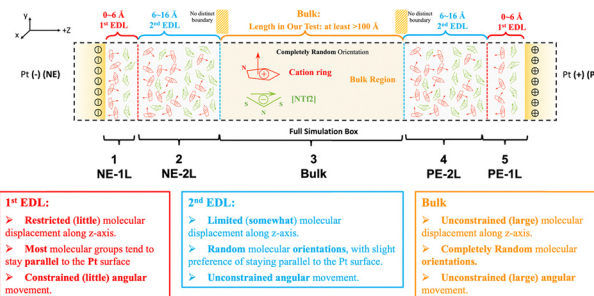
Inbal Offen-Polak, Hilla Ayali Aviram, Adan Hijaze, Thierry K. Slot and David Eisenberg*



10962

[Bmpy] or [Bmim]: which is better for H₂ sensing?

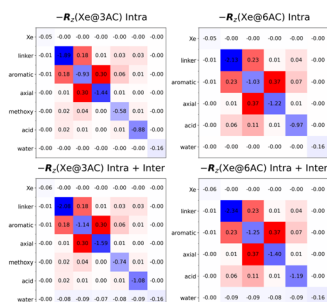
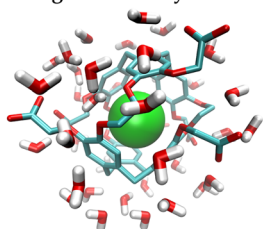
Yining He, Tobias Glossmann, Xiangqun Zeng and Wei Lai*



RESEARCH PAPERS

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Generalised MD modelling of DD-driven nuclear magnetisation dynamics.

Multiscale modelling of nuclear magnetisation dynamics: spin relaxation, polarisation transfer and chemical exchange in ^{129}Xe @cryptophane(aq) structures

Perttu Hilla* and Juha Vaara

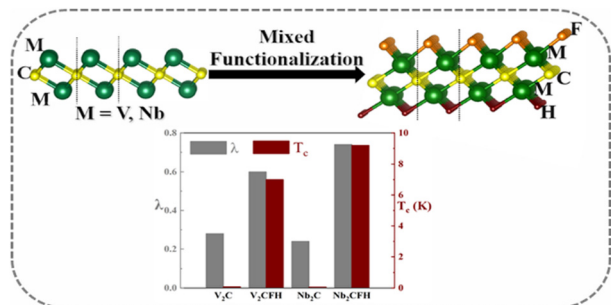
11000



Identifying efficiency-loss pathways in triplet–triplet annihilation upconversion systems

Abhishek Kalpattu, Daniel E. Falvey and John T. Fourkas*

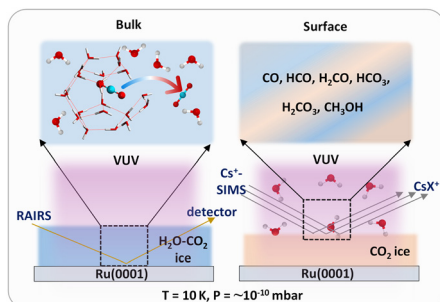
11017



Mixed functionalization as a pathway to induce superconductivity in MXenes: vanadium and niobium carbide

Prarena Jamwal, Rajeev Ahuja and Rakesh Kumar*

11025

Ultraviolet photolysis of CO_2 clathrate hydrate and $\text{H}_2\text{O}-\text{CO}_2$ mixed ice under ultrahigh vacuum

Gaurav Vishwakarma, Bijesh K. Malla, Soham Chowdhury, Jyotirmoy Ghosh, Rabin Rajan J. Methikkalam, Rajnish Kumar* and Thalappil Pradeep*

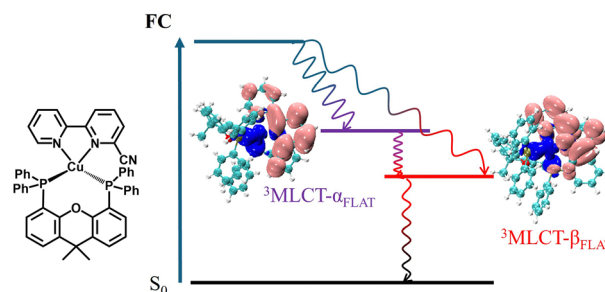


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11036

Effect of the back skeleton ligand on the ultrafast excited-state dynamics of Cu(I) cyano substituted bipyridine complexes

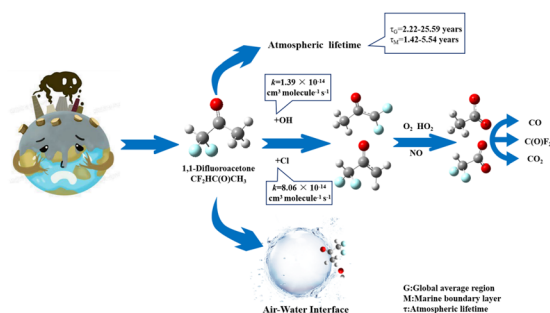
Guanzhi Wu, Qingxue Li, Jinglin Chen* and Wenkai Zhang*



11044

Uncovering the degradation kinetics and mechanisms of difluoroacetone in the atmosphere and at the air–water interface by the OH radical and Cl atom: a theoretical investigation

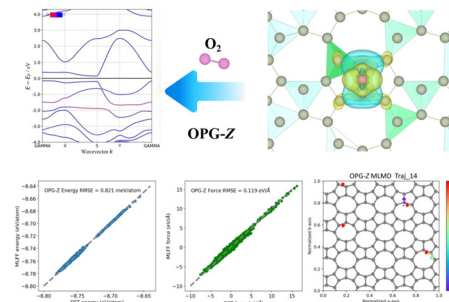
Xiao-Ming Song, Wan-Ying Yu, Ting-Ting Meng, Tai-Xing Chi, Xiang-Huan Liu, Shuang Ni,* Feng-Yang Bai* and Zhen Zhao



11056

Unveiling the oxidation mechanisms of octa–penta graphene: a multidimensional exploration from first-principles to machine learning

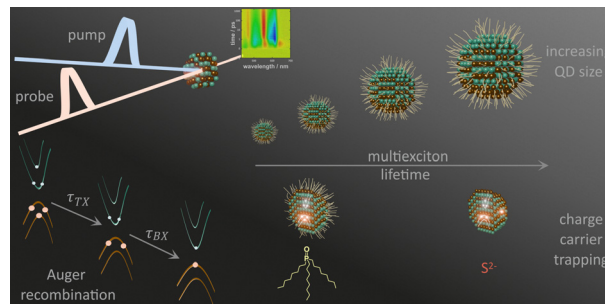
Chenyi Zhou, Rubin Huo, Boyi Situ, Zihan Yan, Yusong Tu and Zhe Zhang*



11066

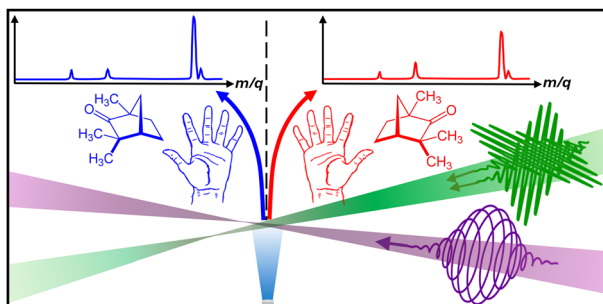
Tuning high-order multiexciton properties of colloidal CdSe quantum dots via size and surface modification

Raktim Baruah, Krishan Kumar, Jan Dellith and Maria Wächtler*



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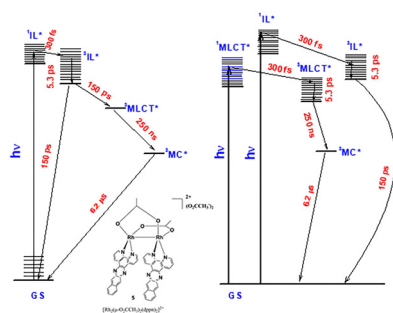
11079



Quantum control of photoion circular dichroism using orthogonal laser beams

Jason B. Greenwood* and Leah Donnelly

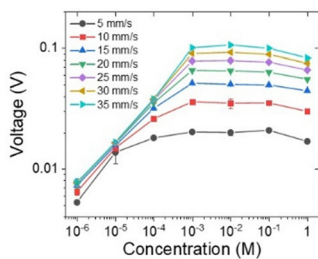
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Photophysics and photochemistry of a prospective light-activated anticancer dirhodium complex

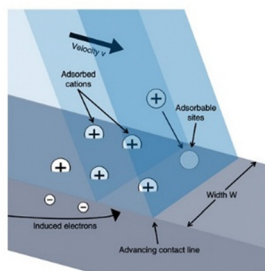
V. A. Meshcheryakova, K. S. Ershov, A. V. Baklanov, A. A. Kokorenko, I. P. Pozdnyakov, Yu. P. Tsentalovich, A. E. Zazulya, D. B. Vasilchenko, E. A. Polyakova, A. A. Melnikov, S. V. Chekalin and E. M. Glebov*

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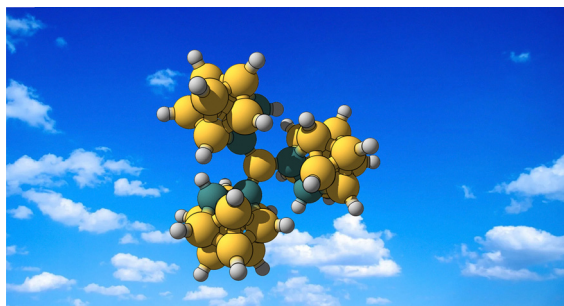


Macroscopic movement of electrolyte-droplet reveals the characteristics of microscopic ion dynamics

Seongmin Park, Hyunbae Cheon, Dongho Shin and Junwoo Park*



11112



Three-fold aromatic boranes: spherical aromaticity in borane *ortho*-carboranes as useful trimer nodes for cluster-based architectures

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

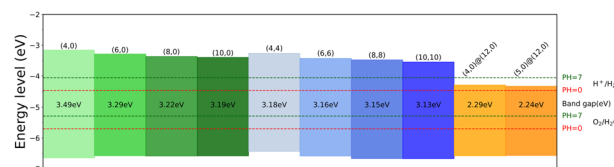


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First principles study of structural and electronic properties of single and double-walled ZnSe nanotubes, toward the photocatalyst application

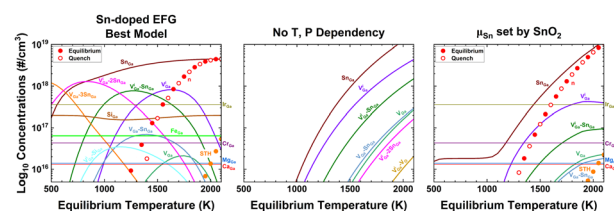
Hao Zuo, Yuqin Zhang,* Guijun Du, Chuxi Ding and Guoying Feng



11129

Quantitative modeling of point defects in β -Ga₂O₃ combining hybrid functional energetics with semiconductor and processes thermodynamics

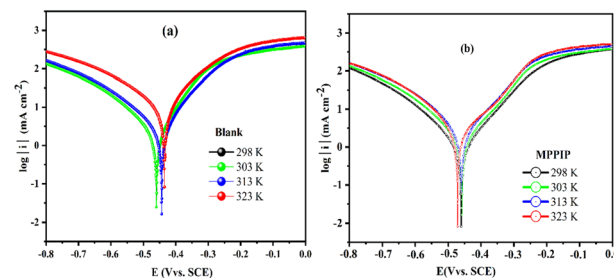
K. A. Arnab, M. Stephens, I. Maxfield, C. Lee, E. Ertekin, Y. K. Frodason, J. B. Varley and M. A. Scarpulla*



11144

Investigating the effectiveness of an imidazopyridine-based compound as an anti-corrosive additive for mild steel in molar hydrochloric acid solutions: a mutual multi-facet experimental and computational approach

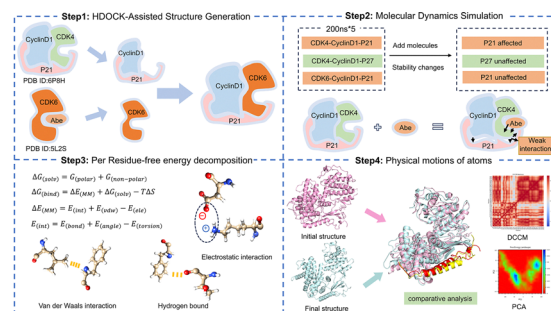
Nouredine Idlahoussaine,* Brahim El Ibrahimi,* Abdelaziz Ait Addi, Walid Daoudi, Rachid Idouhli, Mohammed Lasri, Murat Yilmaz, Mahmoud El Ouadi, Abdelmalik El Aattiaoui and Abdesselam Abouelfida



11162

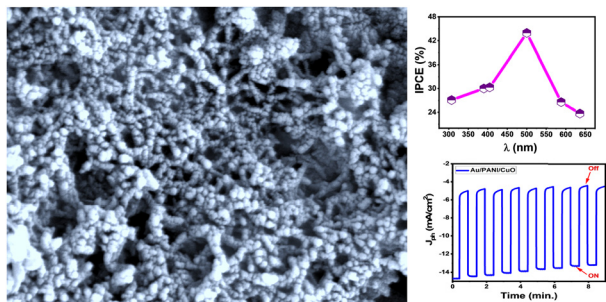
Dynamics insights into CDK4/6–CyclinD1 complex stability modulated by abemaciclib

Yuqing Zhao, Chen Zhuo, Haoquan Liu, Chengwei Zeng, Jiaming Gao, Zhongyi Wei and Yunjie Zhao*



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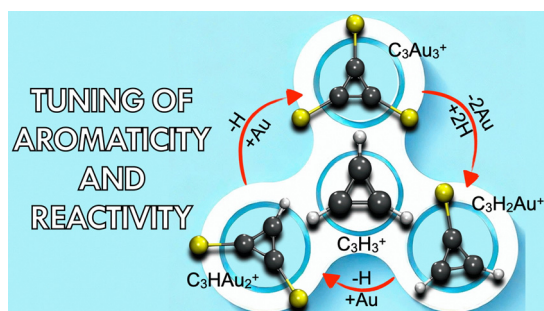
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Fabrication of gold/polyaniline/copper oxide electrode for efficient photoelectrochemical hydrogen evolution

Fahad Abdulaziz, Mohamed Zayed, Salman Latif, Yassin A. Jeilani, Mohamed Shaban, Raja Rama Devi Patel, Hussein A. Elsayed, Mohamed Rabia and Ashour M. Ahmed*

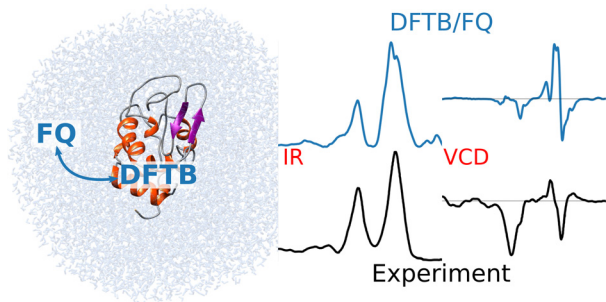
11191



Tuning of aromaticity and reactivity in gold-substituted cyclopropenyl cations

Erick Cerpa,* Alba Vargas-Caamal, Luz Diego, David Arias-Olivares, Diego V. Moreno, Jorge I. Martinez-Araya, Rafael Islas* and Gabriel Merino*

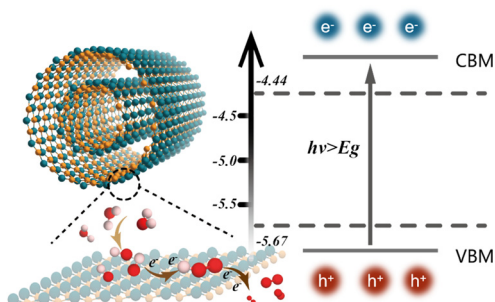
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Modeling infrared and vibrational circular dichroism spectra of complex systems: the DFTB/fluctuating charges route

Piero Lafiosca, Sara Gómez, Luca Melega, Tommaso Giovannini and Chiara Cappelli*

11210



Improved photocatalytic performance of double-walled TeSi nanotubes: a hybrid density functional calculation

Xuan Hui, Hongyu Song, Yingtao Zhu,* Long Zhang, Huanyu Zhao and Weijun Cao*

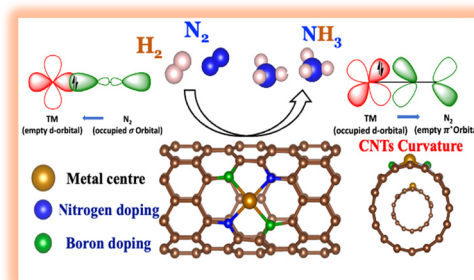


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Tuning surface curvature in B and N co-doped CNT-derived Fe, Ru and Ir catalysts for electrochemical hydrogenation of N_2 to NH_3

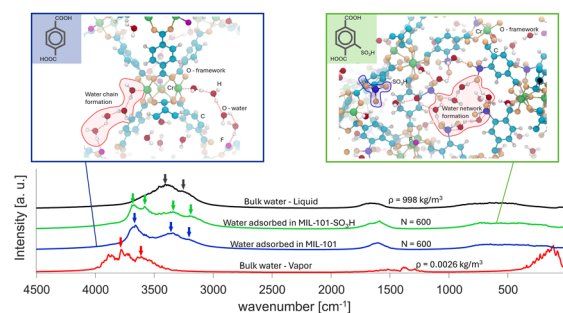
Deewan S. Teja and Bhabani S. Mallik*



11234

Alterations in vibrational spectra of adsorbed water in MIL-101(Cr) and functionalized MIL-101(Cr) using molecular simulations

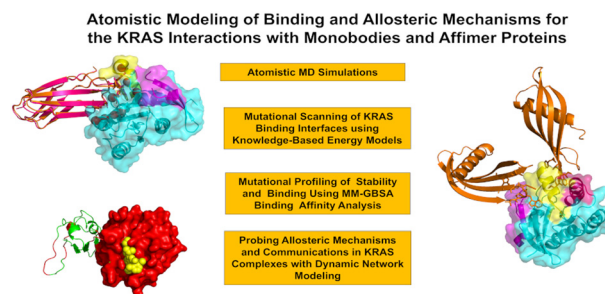
Gunjan Auti, Hao Jiang, Jean-Jacques Delaunay and Hirofumi Daiguji*



11242

Probing binding and allosteric mechanisms of the KRAS interactions with monobodies and affimer proteins: ensemble-based mutational profiling and thermodynamic analysis of binding energetics and allostery reveal diversity of functional hotspots and cryptic pockets linked by conserved communication network

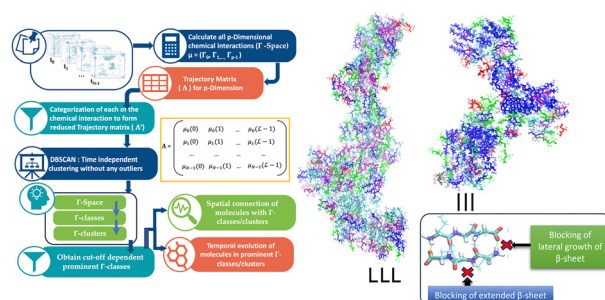
Mohammed Alshahrani, Vedant Parikh, Brandon Foley, Guang Hu and Gennady Verkhivker*



11264

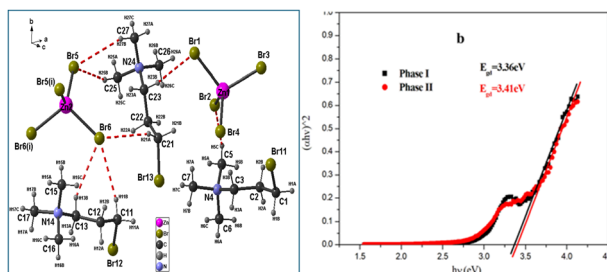
Correlating molecular structures and self-assembly mechanisms *via* temporal analysis of multidimensional chemical interaction space: application to assemblies of isomeric peptides

Sangeeta Das, Rumela Adhikary, Snehamay Bagchi, Argha Chakraborty and Avisek Das*



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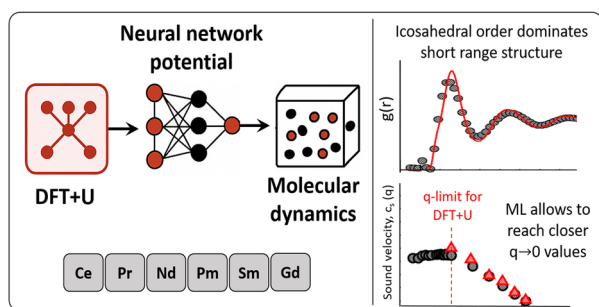
11277



Halogen-regulating synthesis of a novel semiconductor hybrid material $[(\text{CH}_3)_3\text{N}(\text{CH}_2)_3\text{Br}]_2\text{ZnBr}_4$ with high-temperature phase transition

Yosra Rebhi, Imen Dakhloui, Karim Karoui,*
Fadhel Hajlaoui, Nidhal Drissi, Mustapha Zaghrioui,
Cecile Autret, Nathalie Audebrand,
Vincent Dorcet and Fethi Jomni

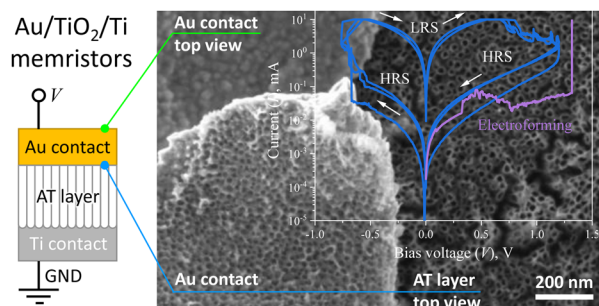
11289



Static, dynamic and electronic properties of some trivalent liquid rare earth metals near melting: *ab initio* and neural network simulations

Beatriz G. del Rio* and Luis E. González

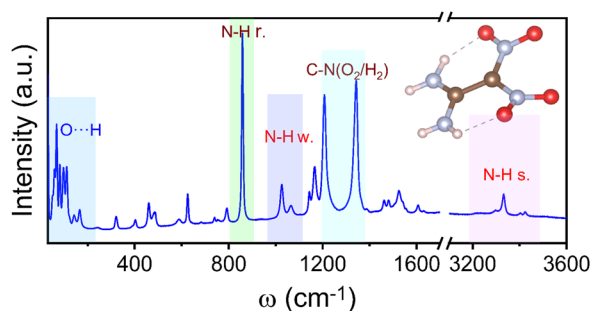
11300



Conduction mechanisms of filamentary resistive switching memristors based on nanoporous and nanotubular titania

Alexander S. Vokhmintsev,* Irina B. Dorosheva,
Robert V. Kamalov and Ilya A. Weinstein

11309



Irregular mechanical and thermal responses of the N–H modes in the FOX-7 energetic material

Jushan Wang, Zhaoyang Zheng, Yangyang Zeng,
Zanhao Wang, Guoyang Yu, Qi-Long Yan,
Huashan Li,* Yanqiang Yang* and Biao Wang

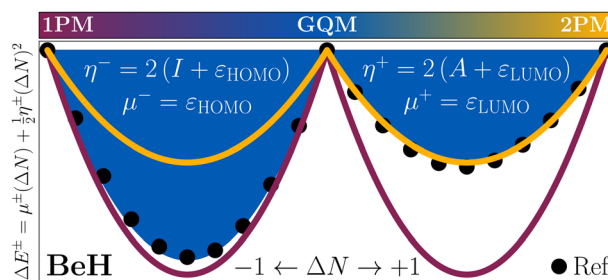


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Generalized quadratic model for charge transfer

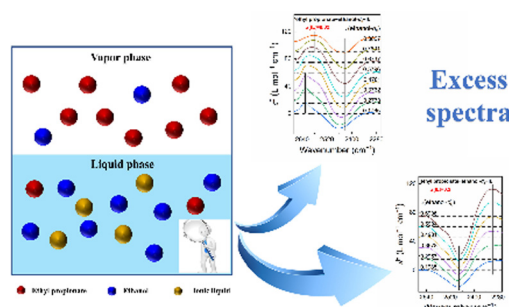
Angel Albavera-Mata, José Luis Gázquez and Alberto Vela*



11331

Mechanism of azeotrope elimination in the ethyl propionate–ethanol system using ionic liquid HMIMOAc as an entrainer: experimental and theoretical insights

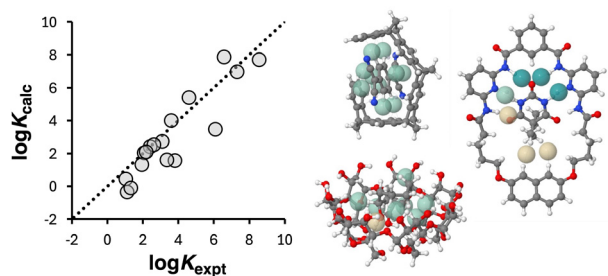
Shuyan Liu, Xiuyu Du, Kuan Ji, Lili Lv and Yu Zhou*



11343

Prediction of solution phase association constants by mapping contact points in intermolecular complexes

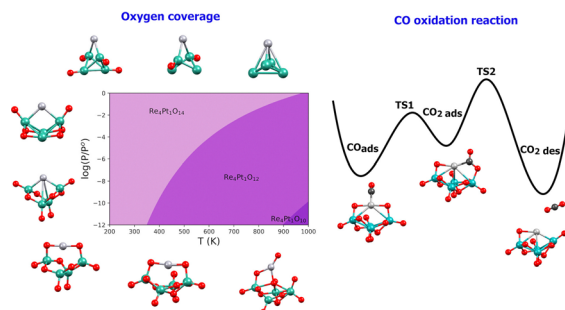
Katarzyna J. Zator and Christopher A. Hunter*



11353

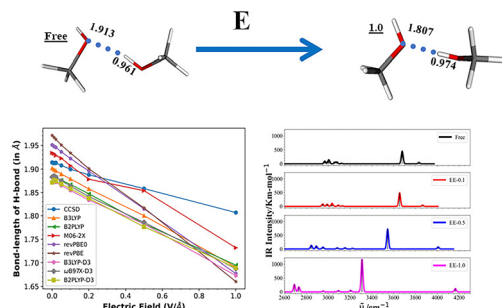
CO oxidation on bimetallic Re–Pt clusters: unraveling the role of oxygen coverage

Andrés Álvarez-García, Ignacio L. Garzón and Luis M. Molina*



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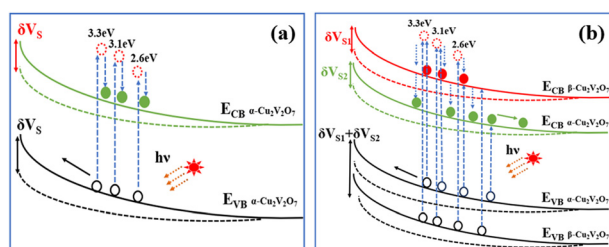
11365



Exploring the effect of external electric fields on the hydrogen bonding of a methanol dimer and fluorinated methanol dimers: a quantum chemical investigation

Shalini Namdev and Satyam Ravi*

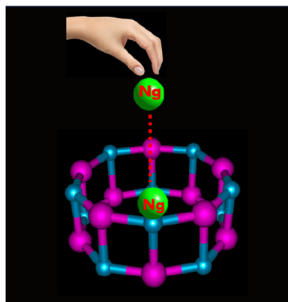
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Constructing heterophase structures of α - $\text{Cu}_2\text{V}_2\text{O}_7$ / β - $\text{Cu}_2\text{V}_2\text{O}_7$ to enhance photovoltaic and photocatalytic properties

Yong Hu, Xiansheng Liu,* Jianjun Tian, Chaoyang Kang, Feng Zhang, Erjun Liang* and Weifeng Zhang*

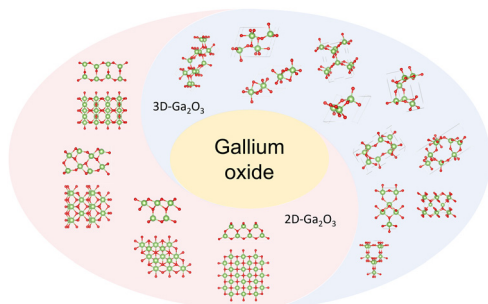
11384



$\text{Ng@M}_{10}\text{H}_{10}$: nobel gas trapping by an alkali hydride cage

Farnaz Yashmin, Kangkan Sarmah, Pankaz K. Sharma* and Ankur K. Guha*

11393



Crystal structure prediction of three- and two-dimensional Ga_2O_3 using a multi-objective differential evolution algorithm

Lei Wang, Danling Wang, Zian Chen, Tao He, Lina Xu,* Xiangju Xu,* Hongping Xiao, Yueyu Zhang* and Guoyong Fang*

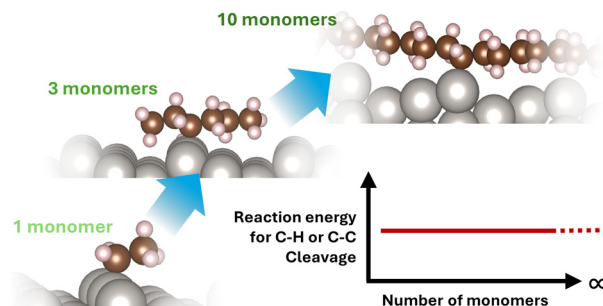


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Theoretical determination of a model molecule for the catalytic upcycling of polyethylene and polypropylene

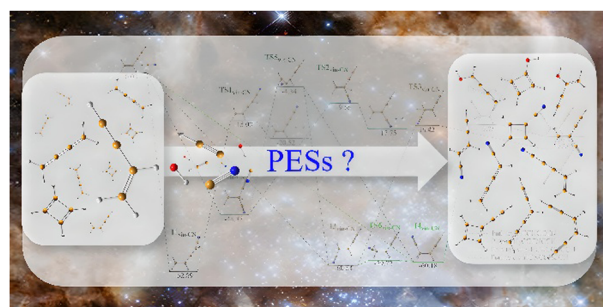
Jessica Ortega-Ramos, Mikael Maraschin, Gerardine G. Botte* and Joseph A. Gauthier*



11413

Formation of hydroxy, cyano and ethynyl derivatives of C₄H₄ isomers in the interstellar medium

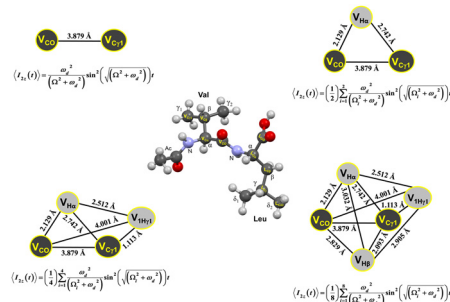
Mario Largo, Miguel Sanz-Novo and Pilar Redondo*



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Modeling dissipative magnetization exchange dynamics in magnetic resonance

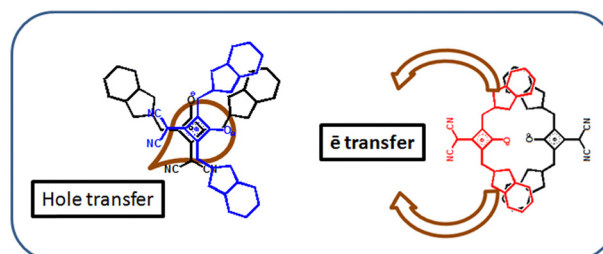
Neelam Sehrawat, Manoj Kumar Pandey* and Ramesh Ramachandran*



11445

Inter- and intra-stacking-influenced charge hopping interactions in core-substituted squaraine dye derivatives: a computational investigation

Rupali R. Deshmukh, Harshada A. Barve and Krishna Chaitanya Gunturu*



CORRECTION

11464

Correction: A weakened Fermi level pinning induced adsorption energy non-charge-transfer mechanism during O₂ adsorption in silicene/graphene heterojunctions

Xuhong Zhao, Haiyuan Chen, Jianwei Wang* and Xiaobin Niu*

