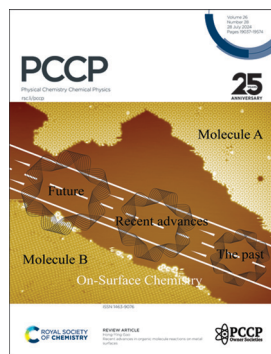


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Cover

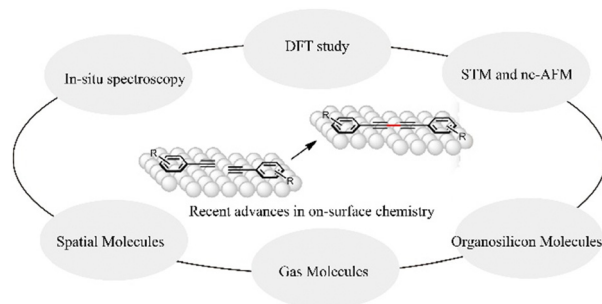
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REVIEWS

19052

Recent advances in organic molecule reactions on metal surfaces

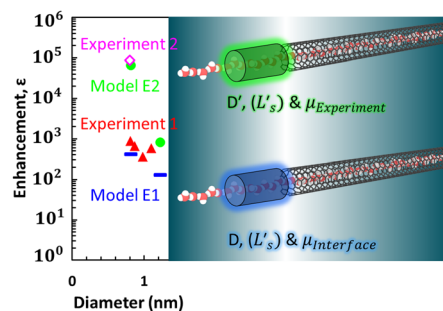
Hong-Ying Gao



19069

Estimating water transport in carbon nanotubes: a critical review and inclusion of scale effects

Kazi Ehsanul Karim, Murat Barisik, Chirodeep Bakli and BoHung Kim*



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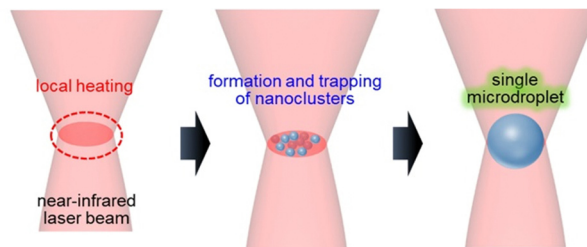
Fundamental questions
Elemental answers

COMMUNICATION

19083

Optical trapping of nanoclusters formed in a temperature-responsive ionic liquid aqueous solution under focused near-infrared laser irradiation

Maho Tanaka, Rai Kobayashi, Yasuyuki Tsuboi and Ken-ichi Yuyama*

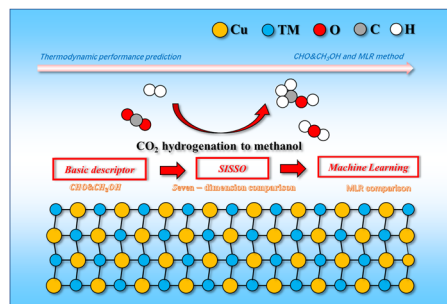


RESEARCH PAPERS

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A systematic theoretical study of CO₂ hydrogenation towards methanol on Cu-based bimetallic catalysts: role of the CHO&CH₃OH descriptor in thermodynamic analysis

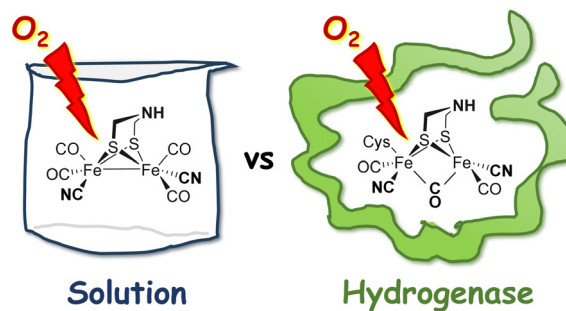
Huang Qin, Hai Zhang,* Kunmin Wu, Xingzi Wang and Weidong Fan



19105

Oxygen sensitivity of [FeFe]-hydrogenase: a comparative study of active site mimics inside vs. outside the enzyme

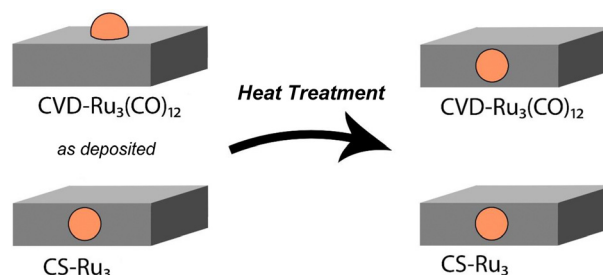
Shanika Yadav, Rieke Haas, Esma Birsan Boydas, Michael Roemelt, Thomas Happe, Ulf-Peter Apfel* and Sven T. Stripp*



19117

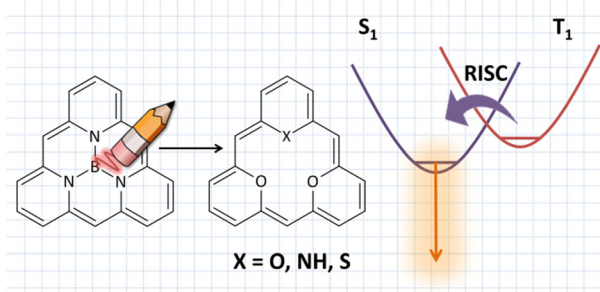
The interaction of size-selected Ru₃ clusters with TiO₂: depth-profiling of encapsulated clusters

Liam Howard-Fabretto, Timothy J. Gorey, Guangjing Li, D. J. Osborn, Sirluck Tesana, Gregory F. Metha, Scott L. Anderson and Gunther G. Andersson*



RESEARCH PAPERS

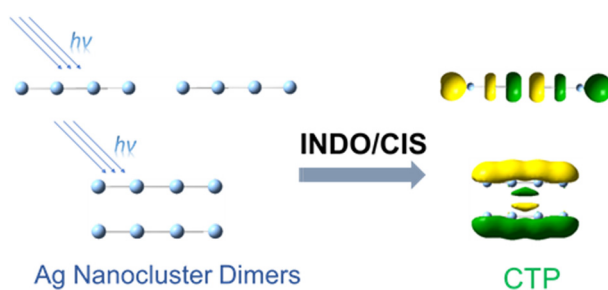
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Computational design of boron-free triangular molecules with inverted singlet–triplet energy gap

Magdalena W. Duszka, Michał F. Rode and Andrzej L. Sobolewski*

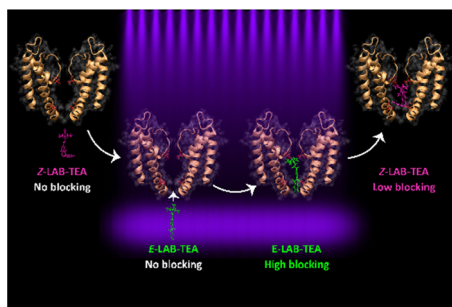
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Quantitative analysis of charge transfer plasmons in silver nanocluster dimers using semiempirical methods

Qiwei Sun, Yavuz S. Ceylan and Rebecca L. M. Gieseking*

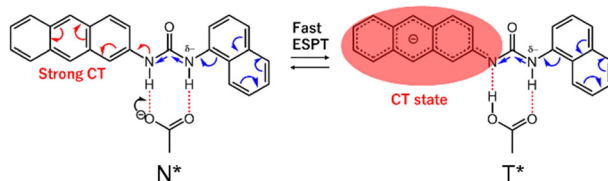
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Deciphering the shape selective conformational equilibrium of *E*- and *Z*-locked azobenzene–tetraethylammonium ion in regulating photo-switchable K^+ -ion channel blocking

Rinsha Cholasseri and Susmita De*

19176



π -Conjugation effects on excited-state intermolecular proton-transfer reactions of anthracene–urea derivatives in the presence of acetate anions

Atsushi Tachibanaki, Toru Matsui and Yoshinobu Nishimura*



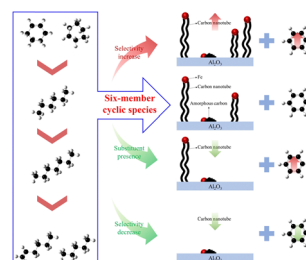
RESEARCH PAPERS

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Role of the hydrocarbon molecular structure in CNT growth on Fe–Al catalysts

Siqi Liu, Xu Hou,* Changchang Tian, Ao Dong, Xinyao Sun, Li Yin,* Jing Huang and Enxian Yuan*

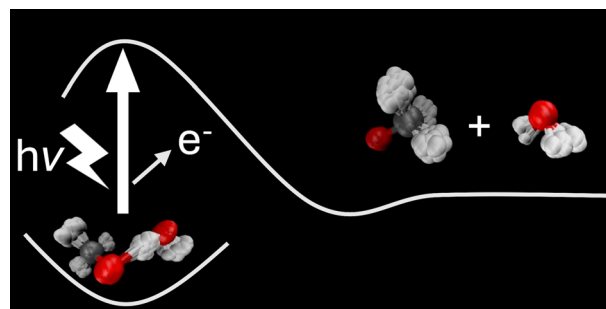
Roles of hydrocarbon molecular structure in CNTs growth on Fe–Al catalyst



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Computational study of the post-transition state dynamics for the OH + CH₃OH reaction probed by photodetachment of the CH₃O[−](H₂O) anion

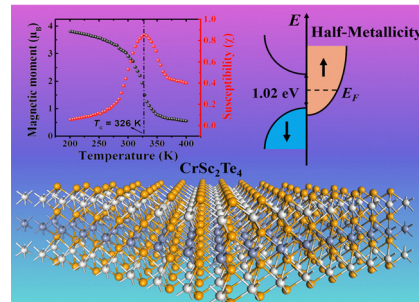
Tatsuhiko Murakami* and Toshiyuki Takayanagi*



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Room-temperature ferromagnetism, half-metallicity and spin transport in monolayer CrSc₂Te₄-based magnetic tunnel junction devices

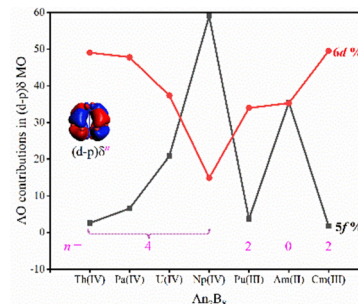
Ruixue Yue, Xuemin Su, Xiaodong Lv,* Bingwen Zhang, Shaolong Su, Haipeng Li, Shaoqiang Guo* and Jian Gong*



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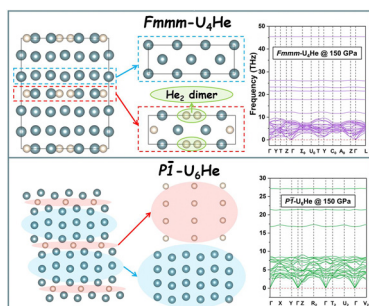
Stability and chemical bonding in a series of inverse sandwich actinide boride clusters (An₂B₈) with δ bonding

Shu-Xian Hu,* Hai-Tao Liu, Zhi-Yu Wei, Bo Wang, Rui-Min Zuo and Ping Zhang



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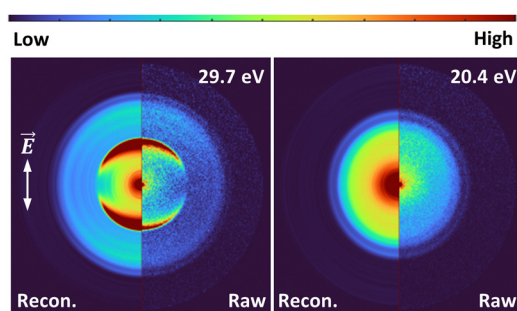
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Theoretical study of the structural and thermodynamic properties of U–He compounds under high pressure

Ye Cao, Hongxing Song,* Xiaozhen Yan, Hao Wang, Yufeng Wang, Fengchao Wu, Leilei Zhang, Qiang Wu* and Huayun Geng*

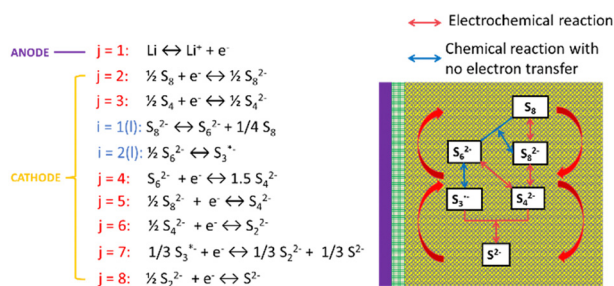
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Valence photoelectron imaging of molecular oxybenzene

Svetlana Tszin,* Loren Ban, Egor Chasovskikh, Bruce L. Yoder and Ruth Signorell*

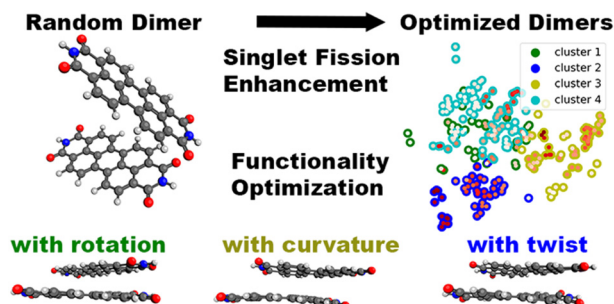
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Reaction kinetics of lithium–sulfur batteries with a polar Li-ion electrolyte: modeling of liquid phase and solid phase processes

Simon Bacon, Shumaila Babar, Matthew Dent, Allan Foster, Joseph Paul Baboo, Teng Zhang, John F. Watts and Constantina Lekakou*

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Functionality optimization for effective singlet fission coupling screening in the full-dimensional molecular and intermolecular coordinate space

Johannes E. Greiner, Anurag Singh and Merle I. S. Röhr*

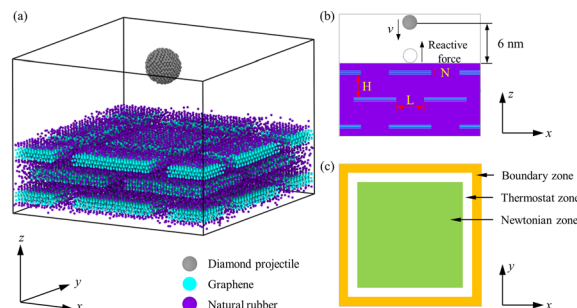


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Unraveling the effects of geometrical parameters on dynamic impact responses of graphene reinforced polymer nanocomposites using coarse-grained molecular dynamics simulations

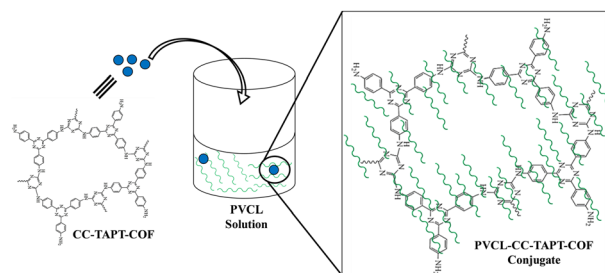
Jianzheng Cui, Fanlin Zeng,* Dahai Wei and Youshan Wang



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Characterization of a conjugate between poly(*N*-vinyl caprolactam) and a triazine-based covalent organic framework as a potential biomaterial

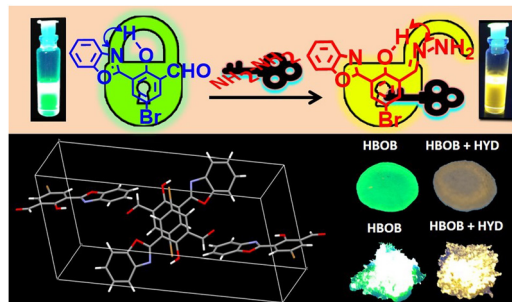
Nitanshu Dhama, Rashmi Prabha, Karan Chaudhary,* Dhanraj T. Masram* and Pannuru Venkatesu*



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Switching of photoinduced proton transfer from one six-membered hydrogen-bonded ring to other: a molecule of hydrazine and pH sensor

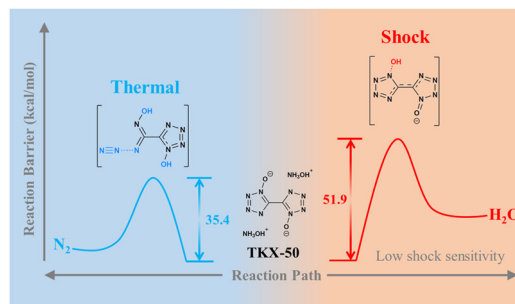
Viki Bhakta and Nikhil Guchhait*



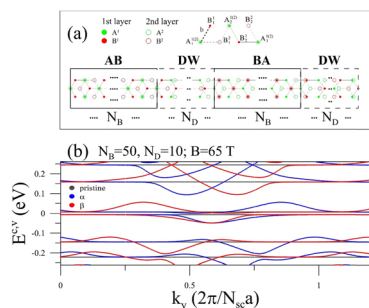
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High energy barrier hydroxyl radical dissociation mechanism of a low shock sensitivity dihydroxylammonium 5,5'-bistetrazole-1,1'-diolate (TKX-50) explosive

Tuo Yang, Danyang Liu,* Kun Yang, Jianying Lu, Bin Zhang, Yiwen Xiao, Kaining Zhang, Junying Wu and Lang Chen



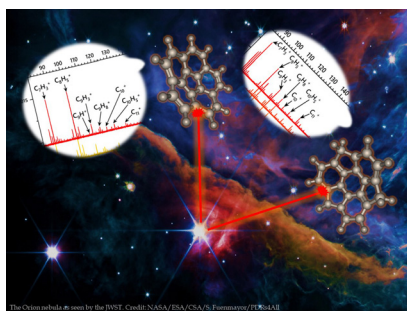
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Unique electronic and optical properties of stacking-modulated bilayer graphene under external magnetic fields

Chiun-Yan Lin, Da-We Weng, Chih-Wei Chiu and Godfrey Gumbs*

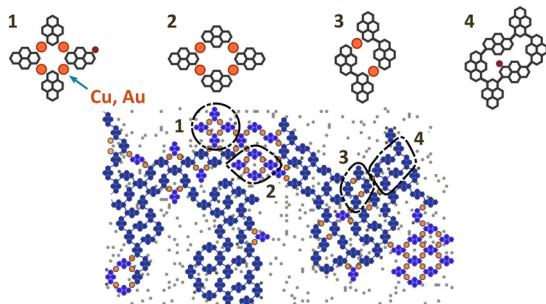
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Photofragmentation of corannulene (C₂₀H₁₀) and sumanene (C₂₁H₁₂) cations in the gas phase and their astrophysical implications

Pavithraa Sundararajan,* Alessandra Candian, Jerry Kamer, Harold Linnartz and Alexander G. G. M. Tielens

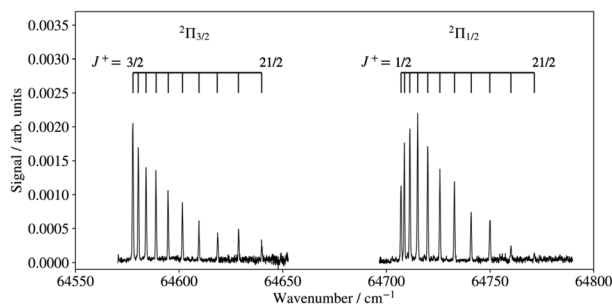
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Theoretical insights into the interplay between metal–organic and covalent bonding in single-layer molecular networks formed by halogen dissociation

Andrius Ibenskas,* Mantas Šimėnas and Evaldas E. Tornau

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Characterisation of the ground $X^+ 2\Pi_{\Omega}$ and first excited $A^+ 2\Sigma^+$ electronic states of MgO^+ by high-resolution photoelectron spectroscopy

C. Kreis, J. R. Schmitz and F. Merkt*

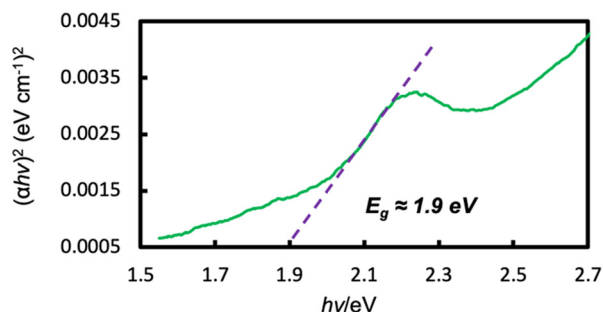


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Periodic DFT calculations to compute the attributes of a quantum material: honeycomb ruthenium trichloride

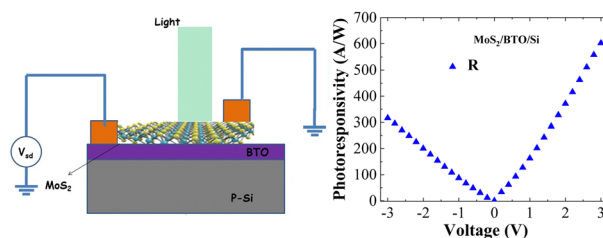
Ashlyn M. Koval, Glen R. Jenness, Timothy C. Schutt,*
Gilbert K. Kosgei, P. U. Ashvin I. Fernando and
Manoj K. Shukla*



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Enhanced photodetection through a perovskite BaTiO₃ dielectric in a Si–MoS₂ heterojunction

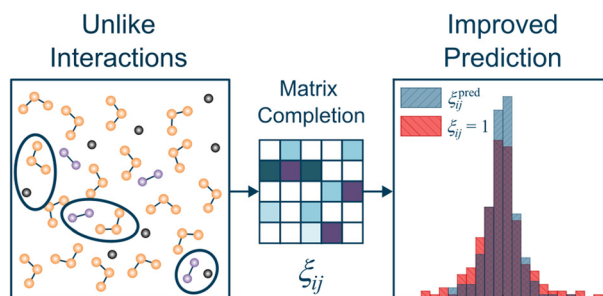
Praloy Mondal



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Prediction of pair interactions in mixtures by matrix completion

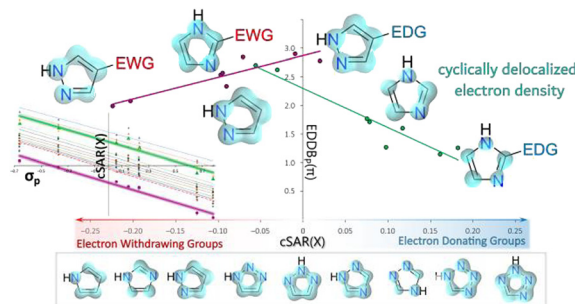
Marco Hoffmann, Nicolas Hayer, Maximilian Kohns,
Fabian Jirasek* and Hans Hasse



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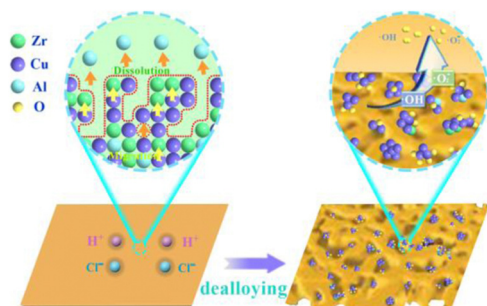
Substituent effects and electron delocalization in five-membered N-heterocycles

Paweł A. Wieczorkiewicz,* Tadeusz M. Krygowski and
Halina Szatyłowicz*



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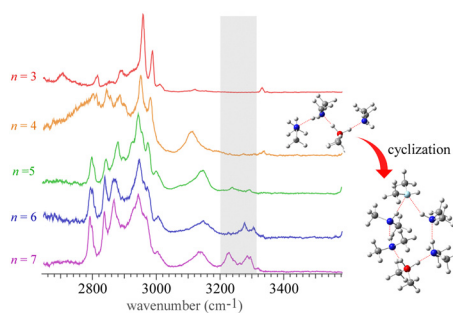
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Surface activation *via* selective dealloying of Cu-based metallic glasses for efficient catalytic behavior

Bowen Zhao, Yichao Wang,* Junmei Zhang, Huan Zhang, Chao Zheng and Zhengwang Zhu*

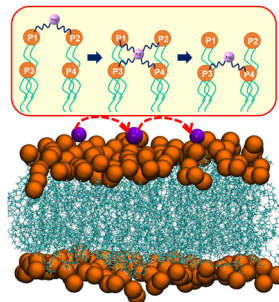
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Hydrogen bond network structures of protonated dimethylamine clusters $H^+(DMA)_n$ ($n = 3-7$)

Atsuya Mizuide and Asuka Fujii*

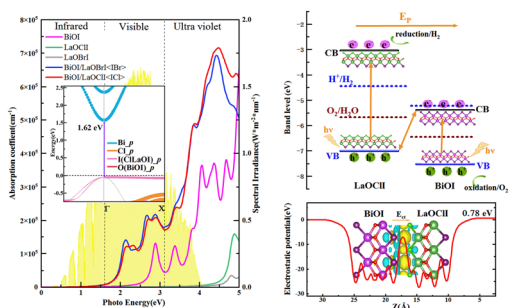
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Lateral diffusion of ions near membrane surface

Subhasish Mallick and Noam Agmon*

19450



Novel BiOI/LaOXI<IX> heterojunction with enhanced visible-light driven photocatalytic performance: unveiling the mechanism of interlayer electron transition

Mengshi Zhou, Chunxiao Zhang,* Chaoyu He, Jin Li, Tao Ouyang, Chao Tang* and Jianxin Zhong

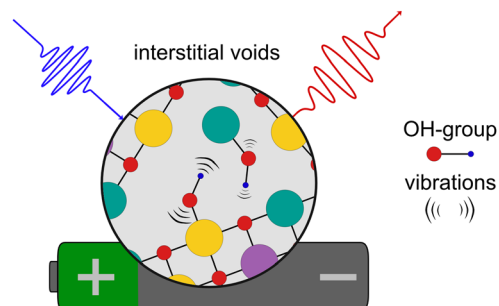


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Vibrationally-resolved RIXS reveals OH-group formation in oxygen redox active Li-ion battery cathodes

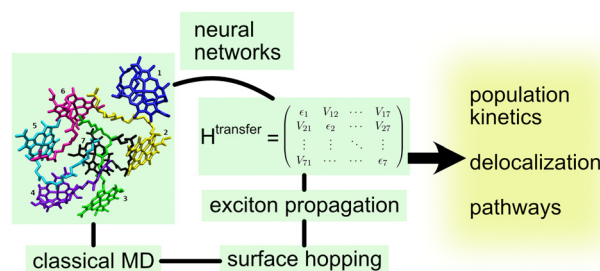
Moritz Hirsbrunner, Anastasiia Mikheenkova, Pontus Törnblom, Robert A. House, Wenliang Zhang, Teguh C. Asmara, Yuan Wei, Thorsten Schmitt, Håkan Rensmo, Soham Mukherjee, Maria Hahlin and Laurent C. Duda*



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Non-adiabatic molecular dynamics simulations provide new insights into the exciton transfer in the Fenna–Matthews–Olson complex

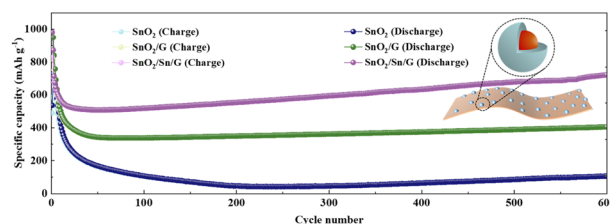
Monja Sokolov, David S. Hoffmann, Philipp M. Dohmen, Mila Krämer, Sebastian Höfener, Ulrich Kleinekathöfer and Marcus Elstner*



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SnO₂/Sn with core–shell structure Schottky heterojunctions loaded in graphene to promote electrochemical reaction kinetics and enable efficient lithium-ion storage

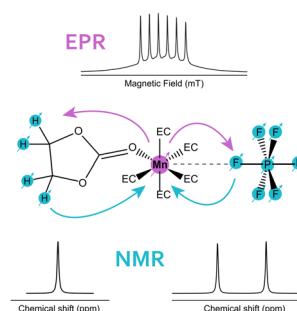
Shujuan Yin, Xueqian Zhang,* Dongdong Liu, Lijuan Zhou, Guangwu Wen, Yishan Wang* and Xiaoxiao Huang*



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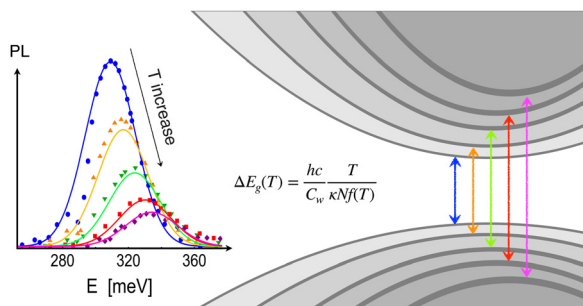
Coordination of dissolved transition metals in pristine battery electrolyte solutions determined by NMR and EPR spectroscopy

Jennifer P. Allen, Conrad Szczuka, Holly E. Smith, Erlendur Jónsson, Rüdiger-A. Eichel, Josef Granwehr and Clare P. Grey*



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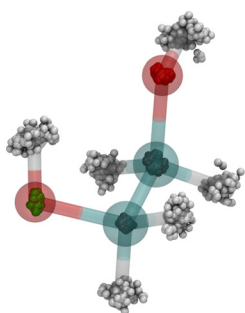
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A statistical theory of the photoluminescence determination of the band gap energy in nano-crystals and layered materials

I. Santamaria-Holek* and A. Pérez-Madrid

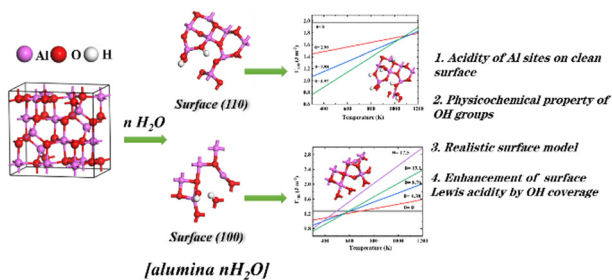
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Nuclear quantum effects in gas-phase ethylene glycol

Mrinal Arandhara and Sai G. Ramesh*

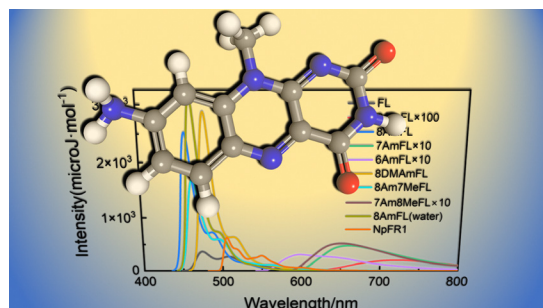
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A thermodynamic model of the surface hydroxylation of γ -Al₂O₃

Ying Ma, Fan Tang, Ziyi Liu, Junqing Li, Haowei Wang, Fan Wu, Dongqi Wang* and An-Hui Lu*

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Lightening flavin by amination for fluorescent sensing

Huimin Guo,* Siyu Liu, Xin Liu* and Lijun Zhang



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Laser-assisted exfoliation of $\text{Ti}_3\text{C}_2\text{T}_x$

Haoze Jiang, Haonan Zhang, Wuning Wei, Mingshun Qi,
Yongpeng Wu and Chenghao Deng*

