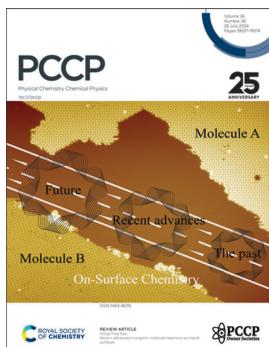


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#### Cover

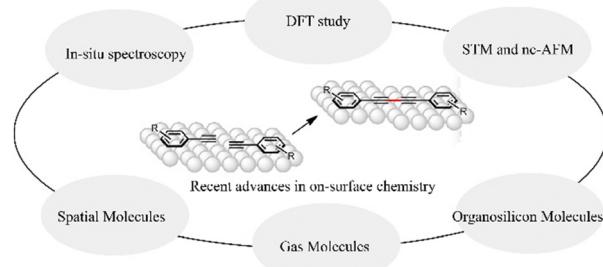
See Hong-Ying Gao,  
pp. 19052–19068.  
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2024, 26, 19052.

### REVIEWS

19052

#### Recent advances in organic molecule reactions on metal surfaces

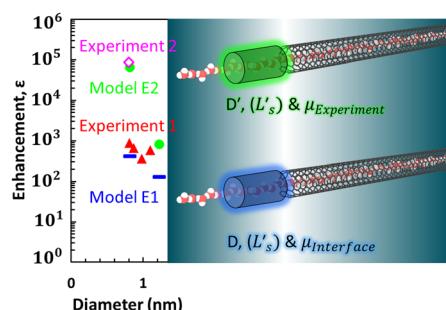
Hong-Ying Gao



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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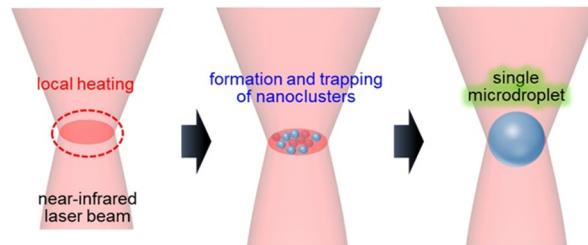
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## COMMUNICATION

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\*

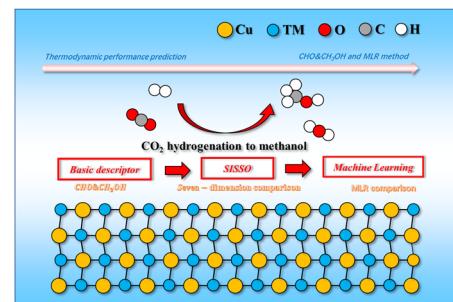


## RESEARCH PAPERS

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**A systematic theoretical study of CO<sub>2</sub> hydrogenation towards methanol on Cu-based bimetallic catalysts: role of the CHO&CH<sub>3</sub>OH descriptor in thermodynamic analysis**

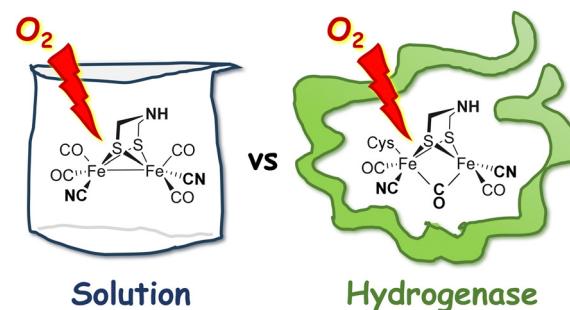
Huang Qin, Hai Zhang,\* Kunmin Wu, Xingzi Wang and Weidong Fan



19105

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

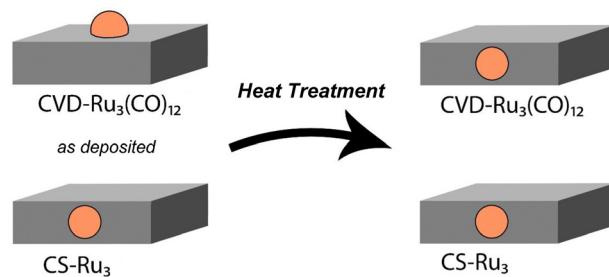
Shanika Yadav, Rieke Haas, Esma Birsen Boydas, Michael Roemelt, Thomas Happe, Ulf-Peter Apfel\* and Sven T. Stripp\*



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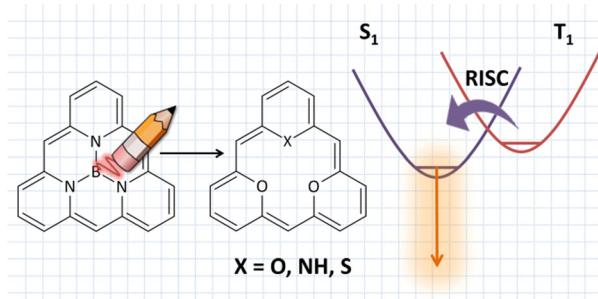
**The interaction of size-selected Ru<sub>3</sub> clusters with TiO<sub>2</sub>: depth-profiling of encapsulated clusters**

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



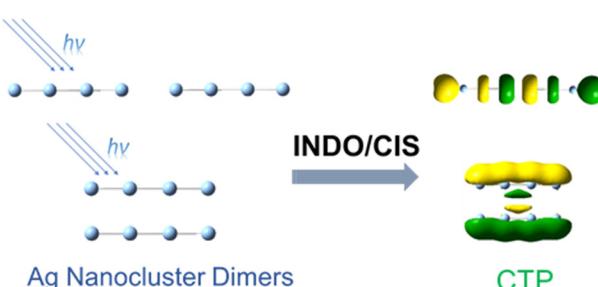
## RESEARCH PAPERS

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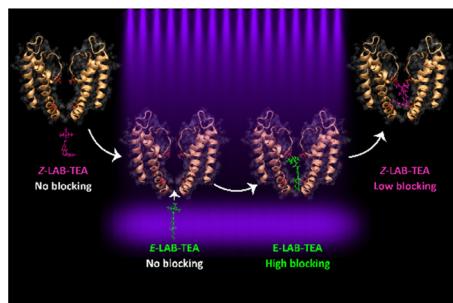
Magdalena W. Duszka, Michał F. Rode and Andrzej L. Sobolewski\*

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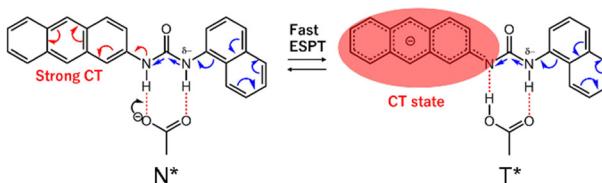
Qiwei Sun, Yavuz S. Ceylan and Rebecca L. M. Giesecking\*

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Rinsha Cholasseri and Susmita De\*

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Atsushi Tachibanaki, Toru Matsui and Yoshinobu Nishimura\*



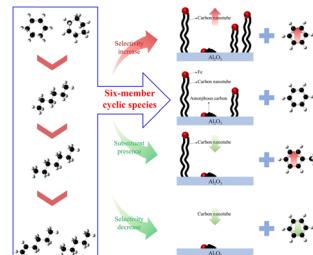
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**Role of the hydrocarbon molecular structure in CNT growth on Fe–Al catalysts**

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

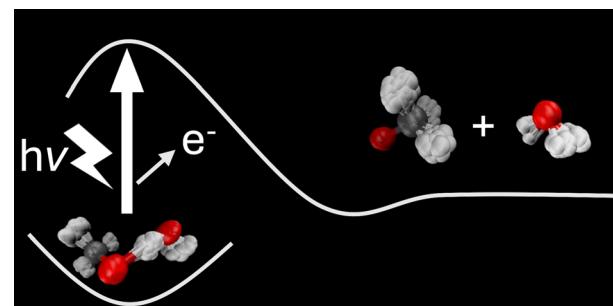
## Roles of hydrocarbon molecular structure in CNTs growth on Fe-Al catalyst



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**Computational study of the post-transition state dynamics for the OH + CH<sub>3</sub>OH reaction probed by photodetachment of the CH<sub>3</sub>O<sup>-</sup>(H<sub>2</sub>O) anion**

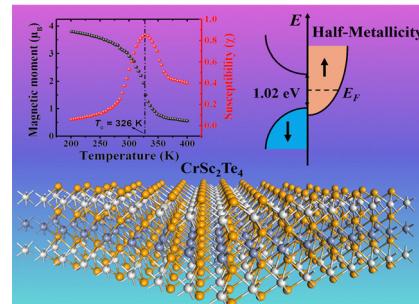
Tatsuhiro Murakami\* and Toshiyuki Takayanagi\*



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**Room-temperature ferromagnetism, half-metallicity and spin transport in monolayer CrSc<sub>2</sub>Te<sub>4</sub>-based magnetic tunnel junction devices**

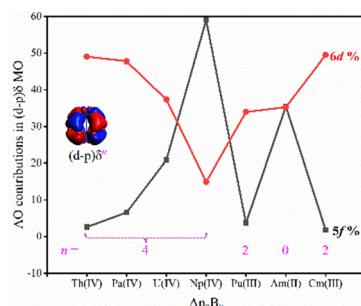
Ruixue Yue, Xuemin Su, Xiaodong Lv,\* Bingwen Zhang, Shaolong Su, Haipeng Li, Shaoqiang Guo\* and Jian Gong\*



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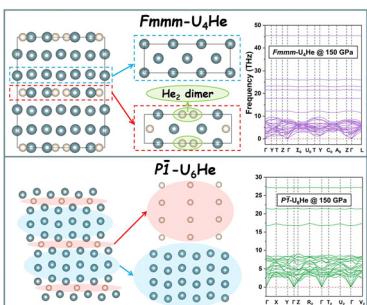
**Stability and chemical bonding in a series of inverse sandwich actinide boride clusters (An<sub>2</sub>B<sub>8</sub>) with δ bonding**

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



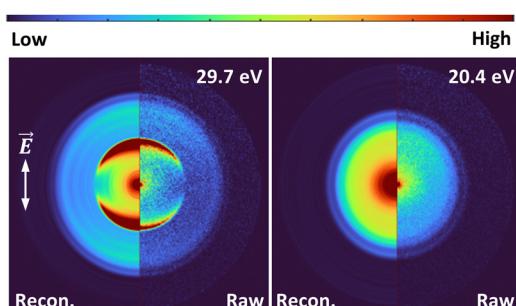
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**Theoretical study of the structural and thermodynamic properties of U-He compounds under high pressure**

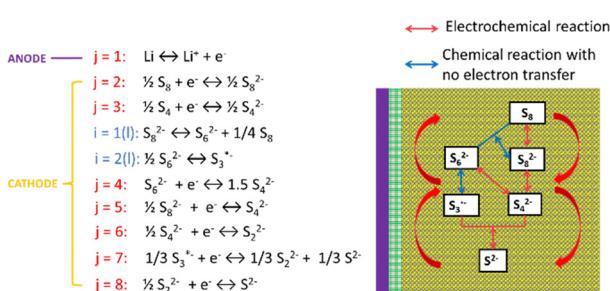
Ye Cao, Hongxing Song,\* Xiaozhen Yan, Hao Wang, Yufeng Wang, Fengchao Wu, Leilei Zhang, Qiang Wu\* and Huayun Geng\*

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**Valence photoelectron imaging of molecular oxybenzone**

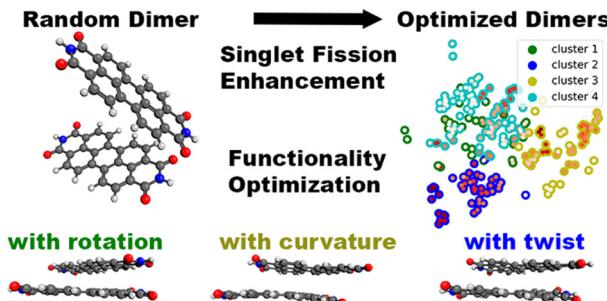
Svetlana Tsizin,\* Loren Ban, Egor Chasovskikh, Bruce L. Yoder and Ruth Signorell\*

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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\*

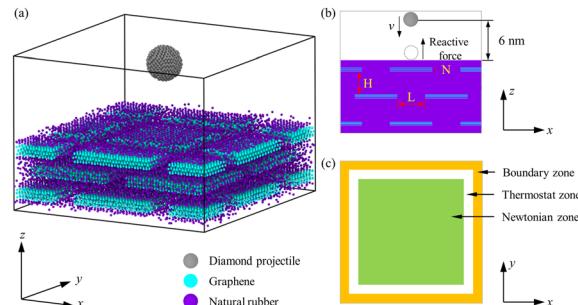


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**Unraveling the effects of geometrical parameters on dynamic impact responses of graphene reinforced polymer nanocomposites using coarse-grained molecular dynamics simulations**

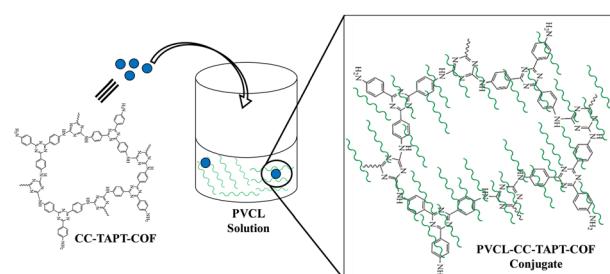
Jianzheng Cui, Fanlin Zeng,\* Dahai Wei and Youshan Wang



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

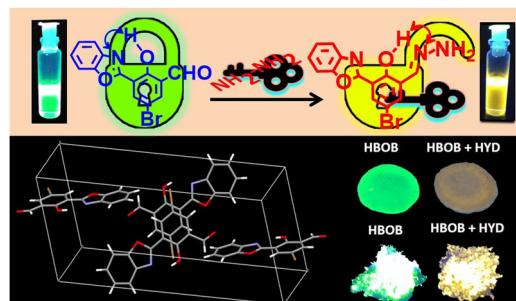
Nitanshu Dhami, Rashmi Prabha, Karan Chaudhary,\* Dhanraj T. Masram\* and Pannuru Venkatesu\*



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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**

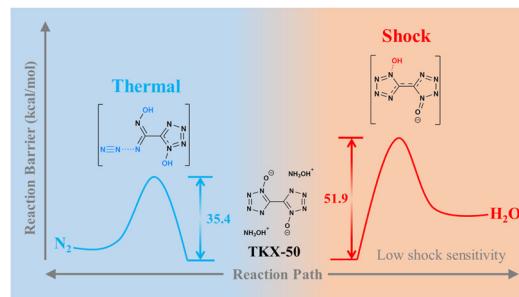
Viki Bhakta and Nikhil Guchhait\*



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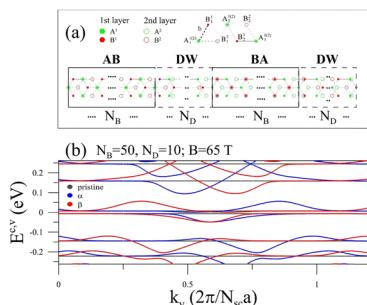
**High energy barrier hydroxyl radical dissociation mechanism of a low shock sensitivity dihydroxylammonium 5,5'-bistetrazole-1,1'-diolate (TKX-50) explosive**

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



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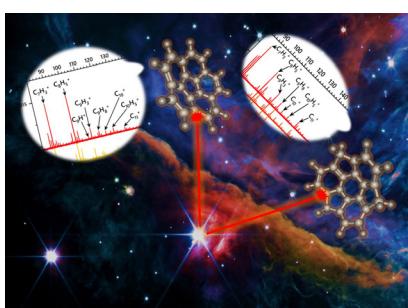
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## Unique electronic and optical properties of stacking-modulated bilayer graphene under external magnetic fields

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

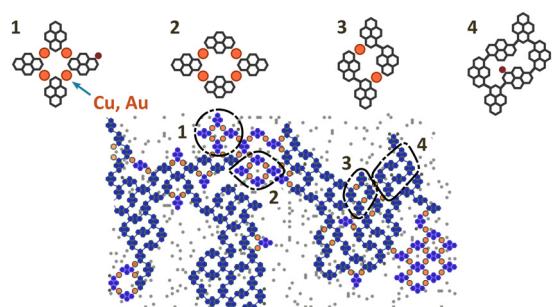
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## Photofragmentation of corannulene ( $C_{20}H_{10}$ ) and sumanene ( $C_{21}H_{12}$ ) cations in the gas phase and their astrophysical implications

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

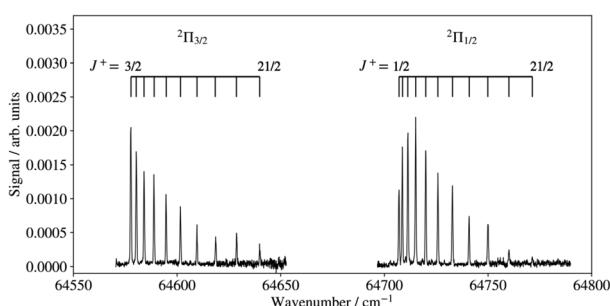
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## Theoretical insights into the interplay between metal–organic and covalent bonding in single-layer molecular networks formed by halogen dissociation

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

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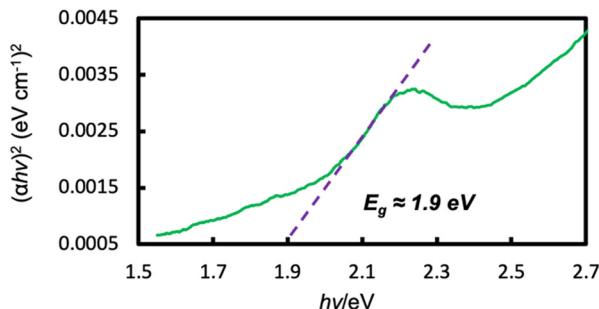


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**Periodic DFT calculations to compute the attributes of a quantum material: honeycomb ruthenium trichloride**

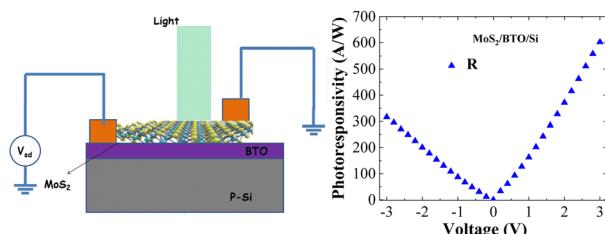
Ashlyn M. Koval, Glen R. Jenness, Timothy C. Schutt,\* Gilbert K. Kosgei, P. U. Ashvin I. Fernando and Manoj K. Shukla\*



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**Enhanced photodetection through a perovskite  $\text{BaTiO}_3$  dielectric in a Si– $\text{MoS}_2$  heterojunction**

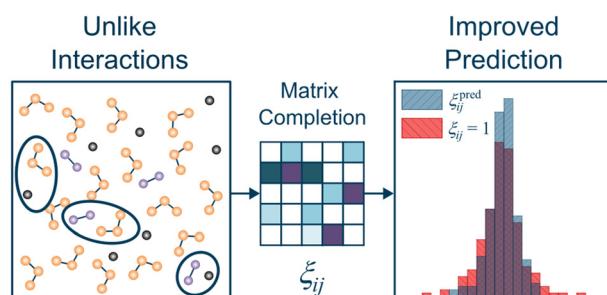
Praloy Mondal



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**Prediction of pair interactions in mixtures by matrix completion**

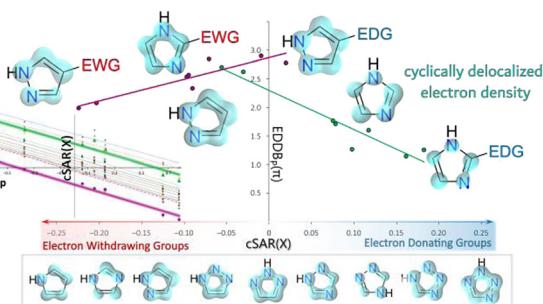
Marco Hoffmann, Nicolas Hayer, Maximilian Kohns, Fabian Jirasek\* and Hans Hasse



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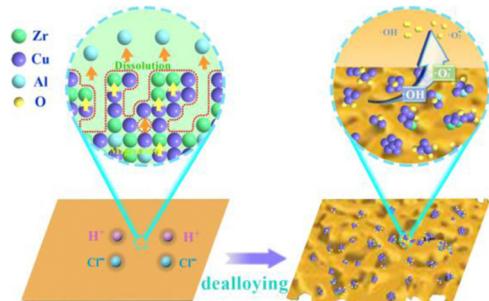
**Substituent effects and electron delocalization in five-membered N-heterocycles**

Paweł A. Wieczorkiewicz,\* Tadeusz M. Krygowski and Halina Szatylowicz\*



## RESEARCH PAPERS

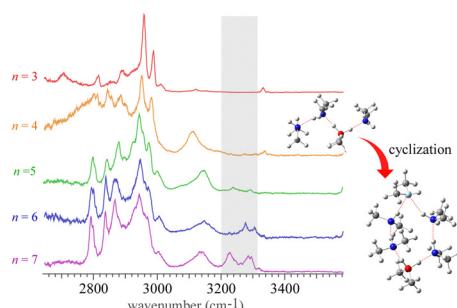
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### Surface activation via selective dealloying of Cu-based metallic glasses for efficient catalytic behavior

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

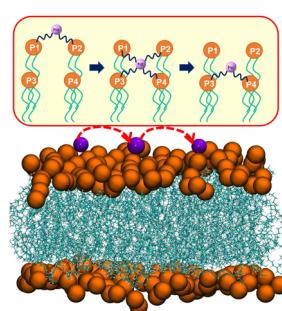
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### Hydrogen bond network structures of protonated dimethylamine clusters $\text{H}^+(\text{DMA})_n$ ( $n = 3-7$ )

Atsuya Mizuide and Asuka Fujii\*

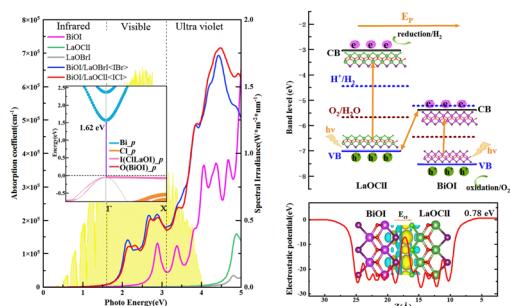
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### Lateral diffusion of ions near membrane surface

Subhasish Mallick and Noam Agmon\*

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### Novel $\text{BiOI}/\text{LaOCl}/\text{IX}$ 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

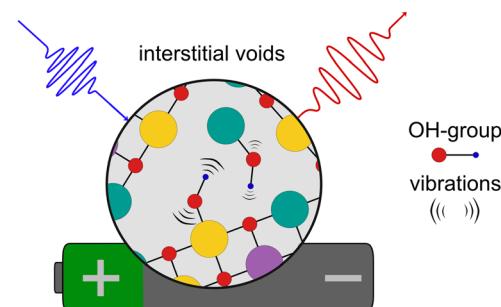


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**Vibrationally-resolved RIXS reveals OH-group formation in oxygen redox active Li-ion battery cathodes**

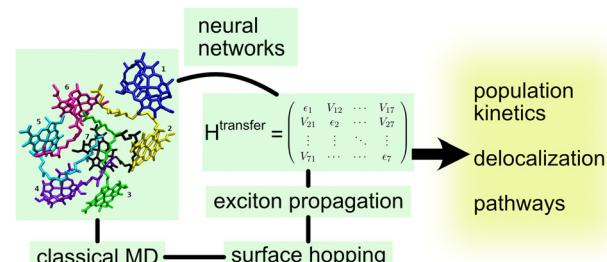
Moritz Hirsbrunner, Anastasiia Mikheenkova, Pontus Törnblom, Robert A. House, Wenliang Zhang, Teguh C. Asmara, Yuan Wei, Thorsten Schmitt, Håkan Rensmo, Soham Mukherjee, Maria Hahlin and Laurent C. Duda\*



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

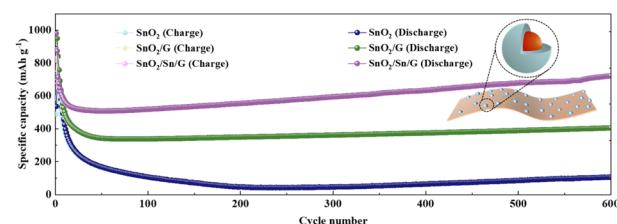
Monja Sokolov, David S. Hoffmann, Philipp M. Dohmen, Mila Krämer, Sebastian Höfener, Ulrich Kleinekathöfer and Marcus Elstner\*



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**SnO<sub>2</sub>/Sn with core–shell structure Schottky heterojunctions loaded in graphene to promote electrochemical reaction kinetics and enable efficient lithium-ion storage**

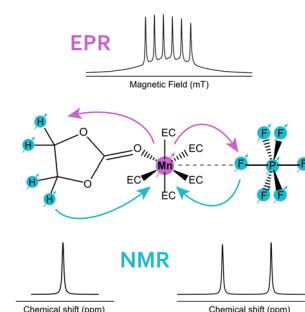
Shujuan Yin, Xueqian Zhang,\* Dongdong Liu, Lijuan Zhou, Guangwu Wen, Yishan Wang\* and Xiaoxiao Huang\*



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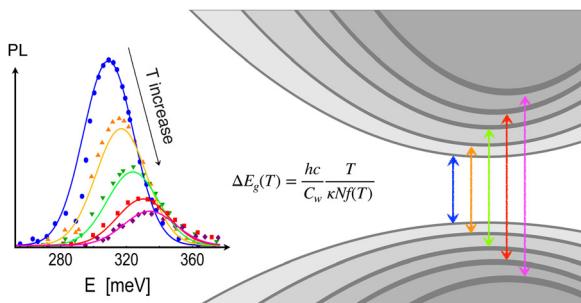
**Coordination of dissolved transition metals in pristine battery electrolyte solutions determined by NMR and EPR spectroscopy**

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



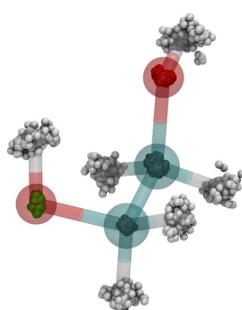
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**A statistical theory of the photoluminescence determination of the band gap energy in nano-crystals and layered materials**

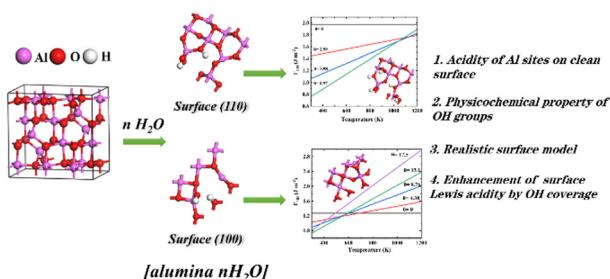
I. Santamaría-Holek\* and A. Pérez-Madrid

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**Nuclear quantum effects in gas-phase ethylene glycol**

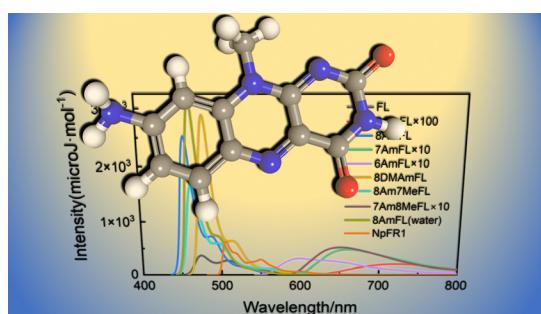
Mrinal Arandhara and Sai G. Ramesh\*

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**A thermodynamic model of the surface hydroxylation of  $\gamma\text{-Al}_2\text{O}_3$** 

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  $Ti_3C_2T_x$** 

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

