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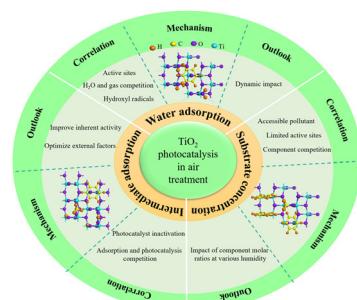
See Aaron D. Wilson et al., pp. 749–759.  
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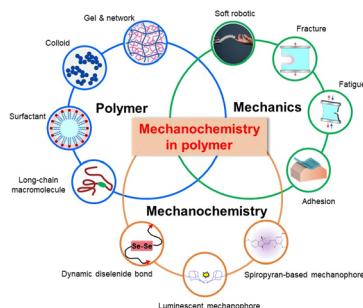
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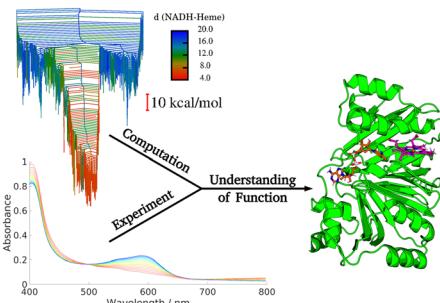
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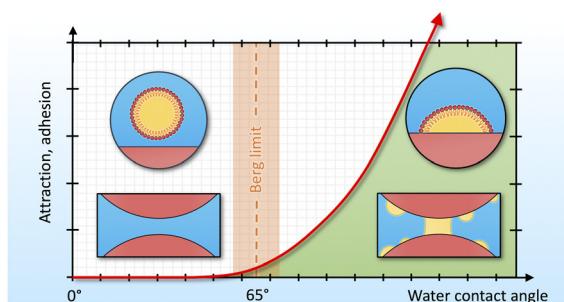
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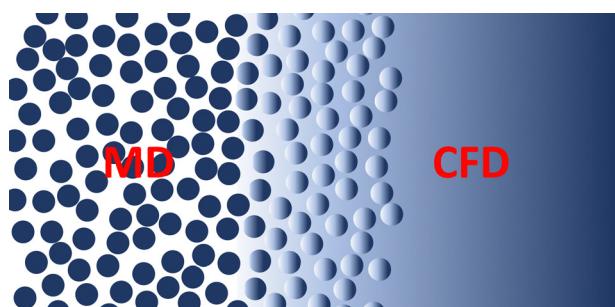
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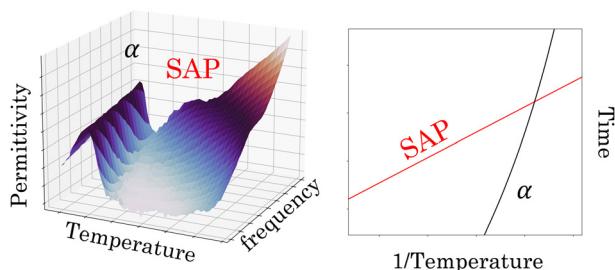


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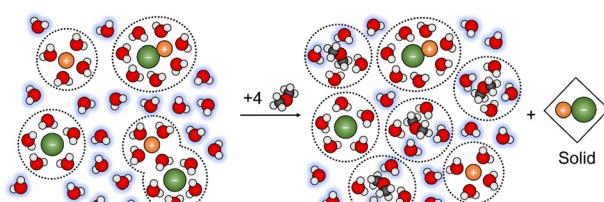
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Federico Caporaletti\* and Simone Napolitano\*



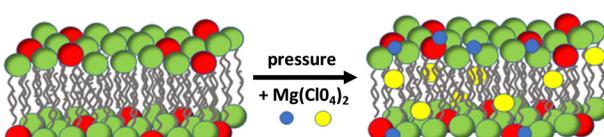
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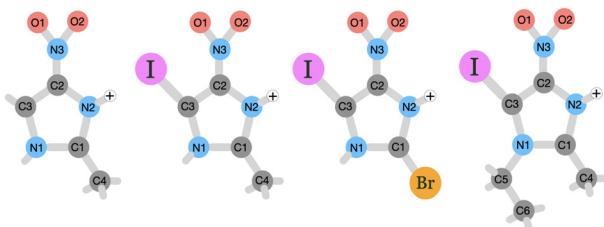
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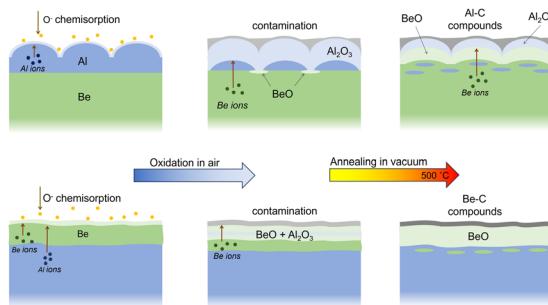
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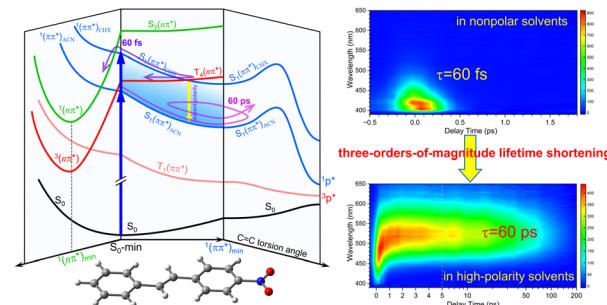


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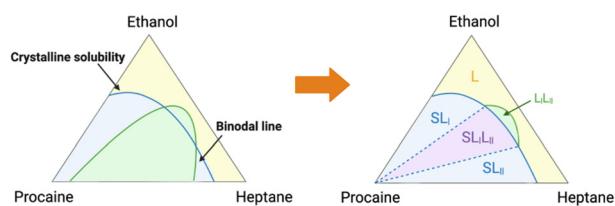
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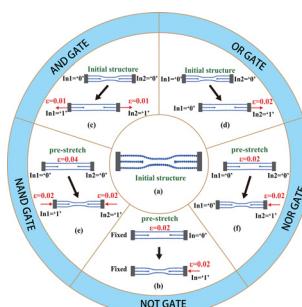
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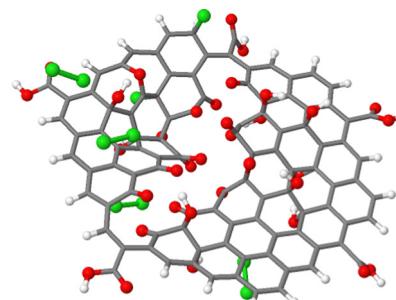
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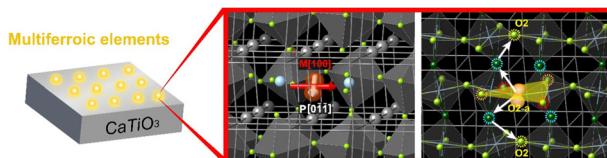
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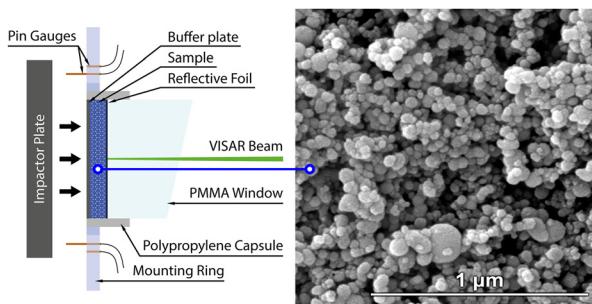
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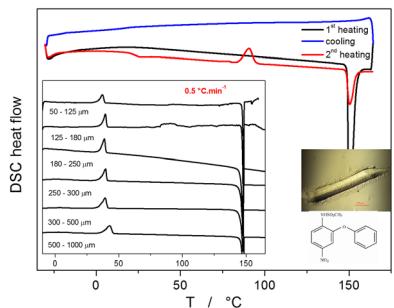
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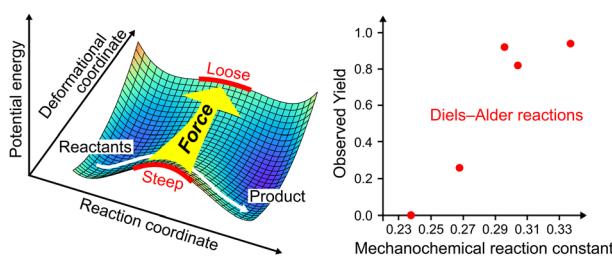
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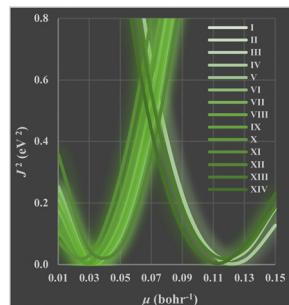


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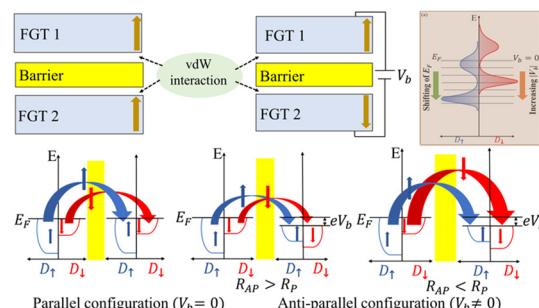
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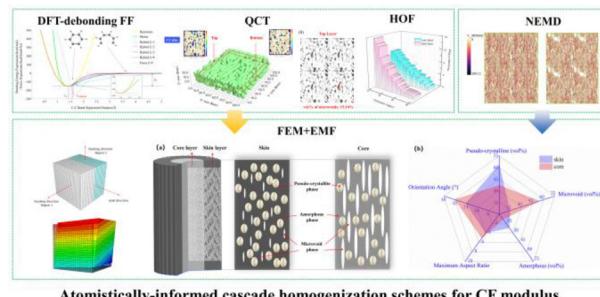
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Anil Kumar Singh, Weibo Gao and Pritam Deb\*



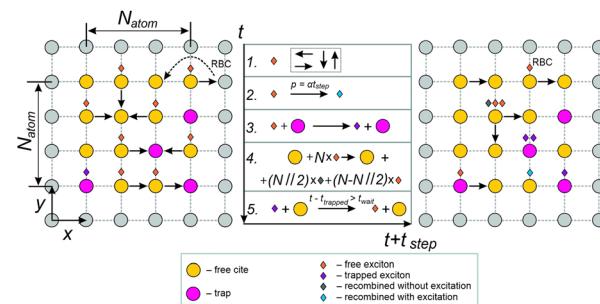
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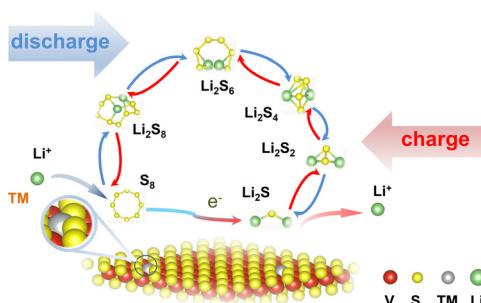
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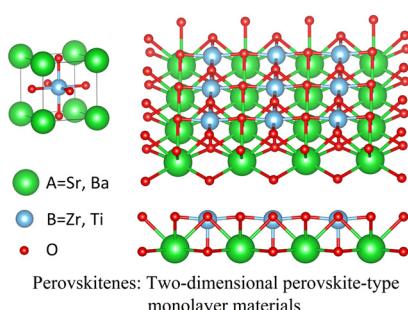
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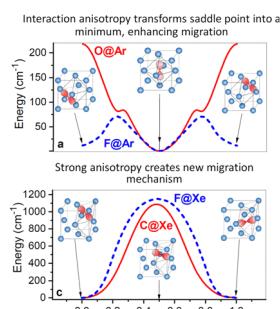
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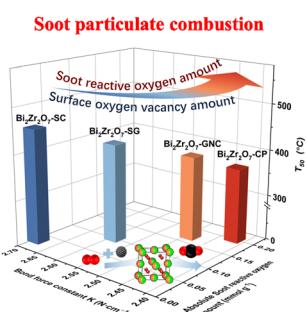
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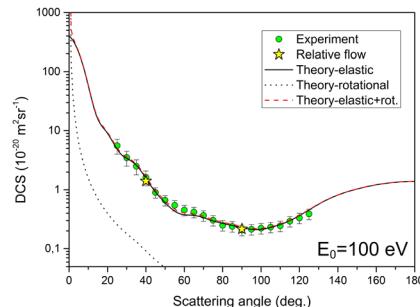


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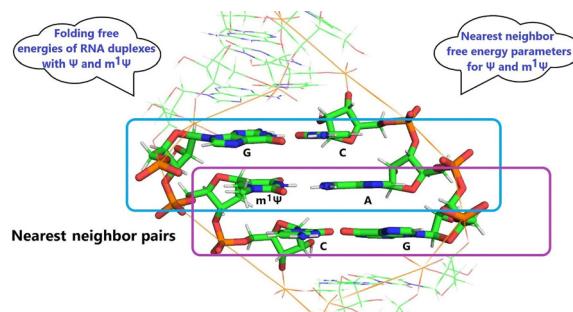
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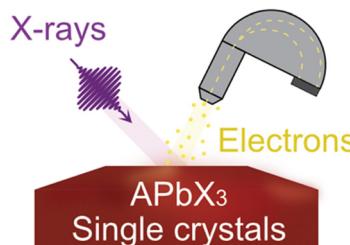


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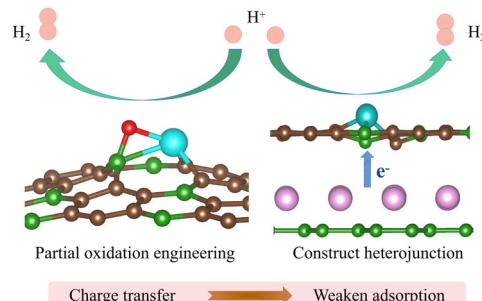


Pb(0) formation  
MAX radiolysis  
Ion migration  
A=MA, FA, Cs  
X=I,Br,Cl

1011

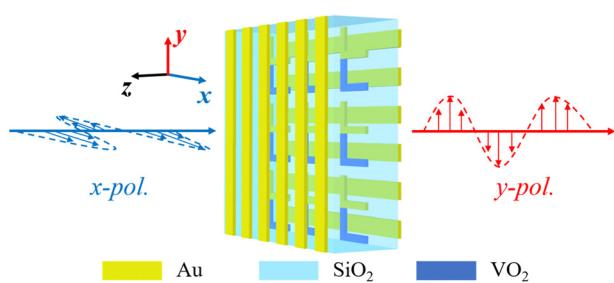
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Liying Pan, Xuxin Kang, Shan Gao\* and Xiangmei Duan\*



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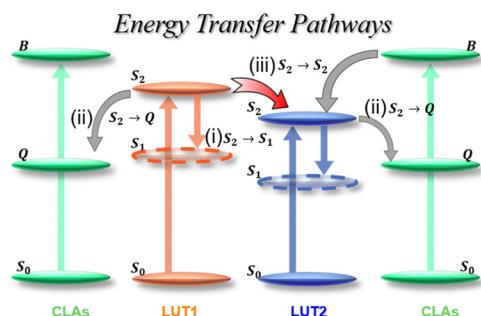
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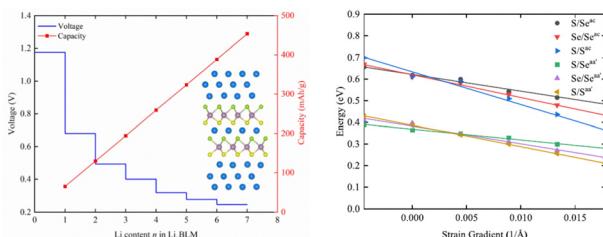
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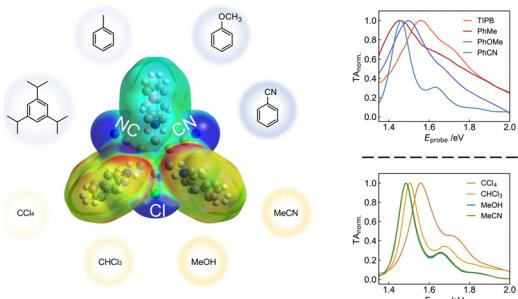
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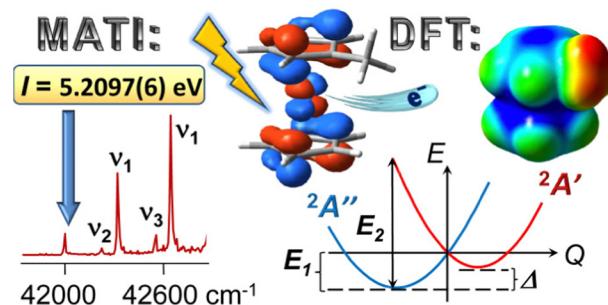


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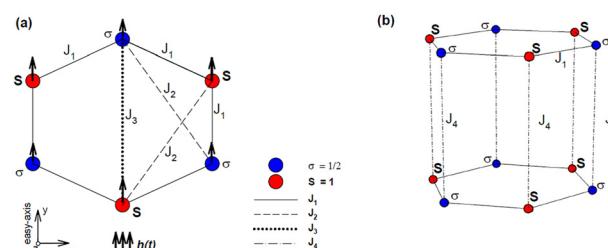
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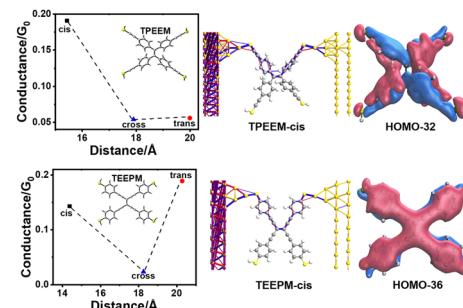
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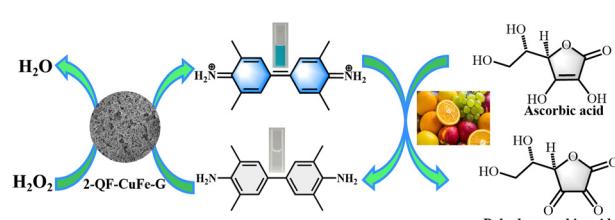
Zhiye Wang, Yunchuan Li\* and Mingjun Sun\*



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Xiao-Juan Wang, Yan Long, Chuan-Wan Wei,\*  
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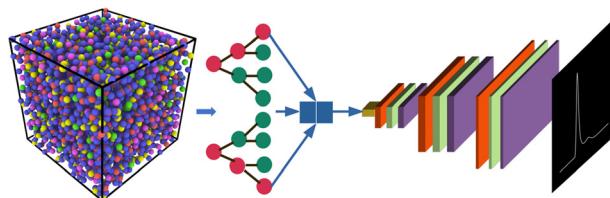
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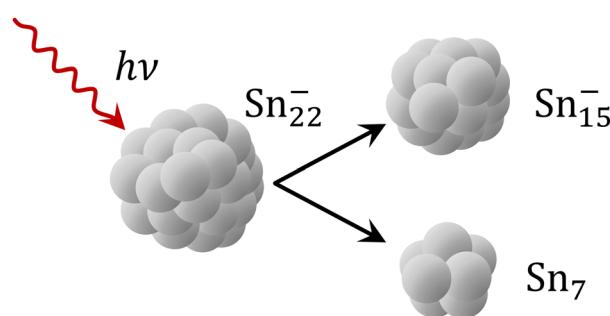
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**Predicting the pair correlation functions of silicate and borosilicate glasses using machine learning**

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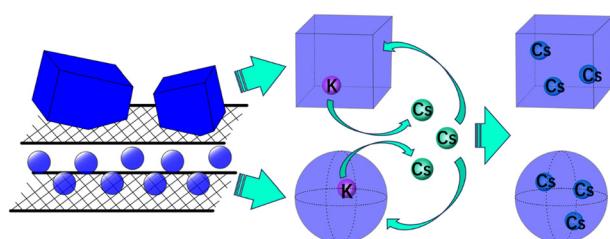
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Alexander Jankowski\*, Paul Fischer, Klavs Hansen and Lutz Schweikhard

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Xindai Li, Kexin Shao, Guangming Xu, Meng Xia, Xinyao Liu, Zhaorong Shang, Fuqiang Fan\* and Junfeng Dou\*

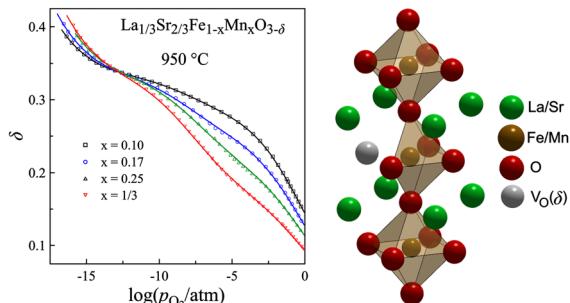


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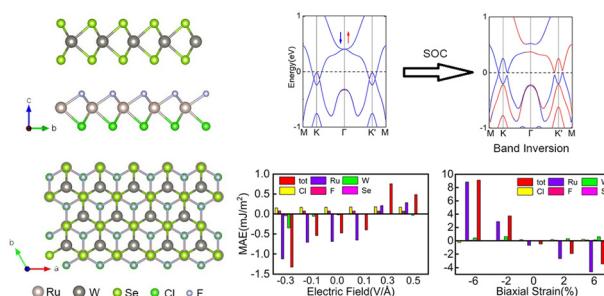
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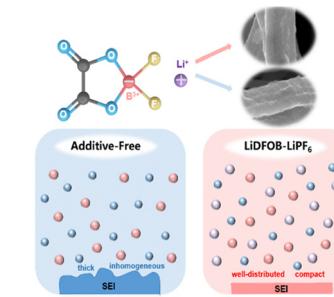
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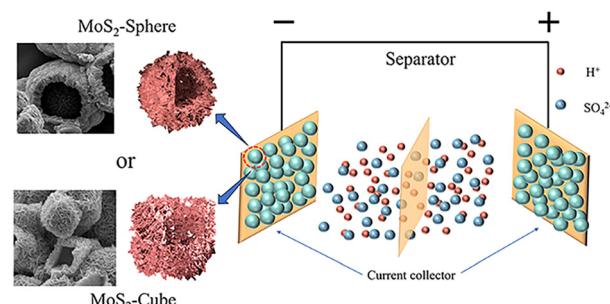
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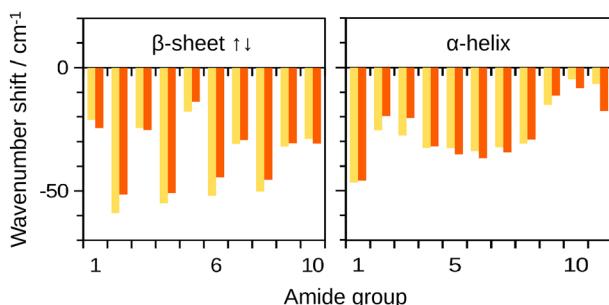
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Yuandong Xu,\* Haoyang Feng, Chaoyang Dong, Yuqing Yang, Meng Zhou, Yajun Wei,\* Hui Guo, Yaqing Wei, Jishan Su, Yingying Ben and Xia Zhang\*



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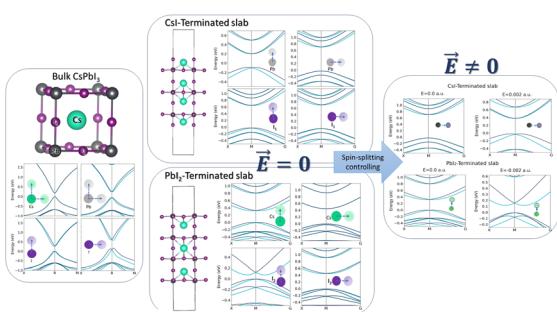
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## Refining protein amide I spectrum simulations with simple yet effective electrostatic models for local wavenumbers and dipole derivative magnitudes

Cesare M. Baronio and Andreas Barth\*

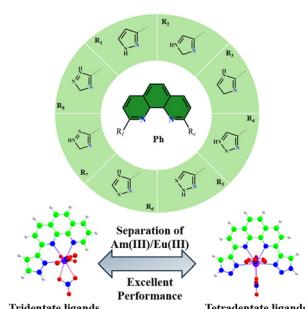
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Safieh Nazari,\* Fatemeh Mohammad Dezashibi and Nadia Babaei Bidmeshki

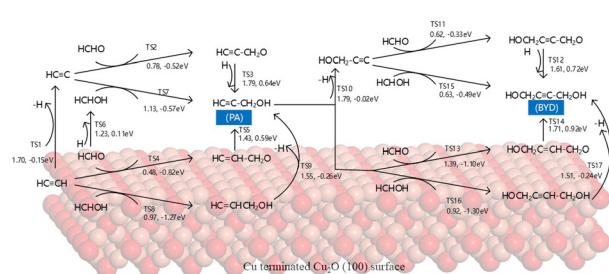
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Minhua Zhang, Qin Yang, Ruishen Li and He Dong\*

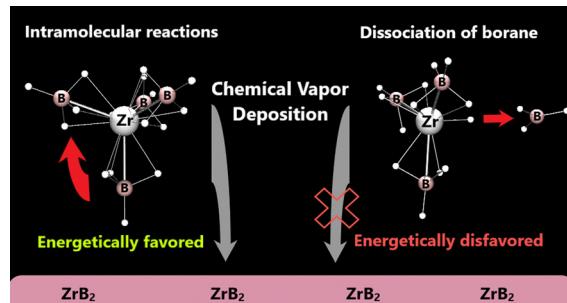


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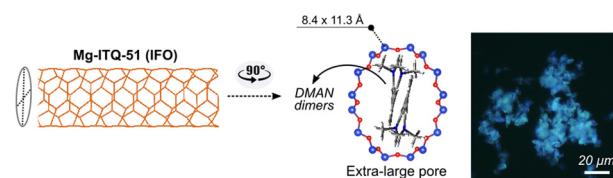
Sergei Prokvolit, Erqian Mao and Thomas G. Gray\*



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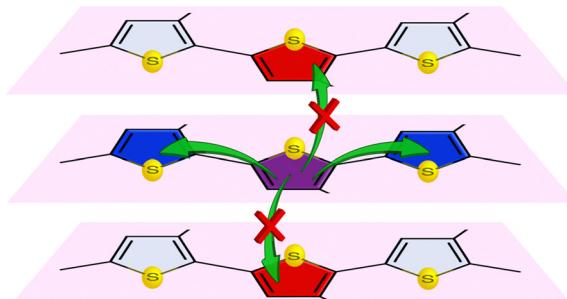
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## X-ray induced ultrafast charge transfer in thiophene-based conjugated polymers controlled by core-hole clock spectroscopy

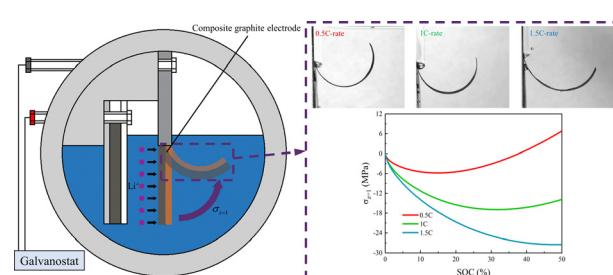
Nicolas Velasquez, Fernanda B. Nunes, Oksana Travnikova, Ilyas Ismail, Renaud Guillemin, Jessica B. Martins, Denis Céolin, Loïc Journel, Laure Fillaud, Dimitris Koulentianos, Chinnathambi Kamal, Ralph Püttner, Maria Novella Piancastelli, Marc Simon, Michael Odelius, Marcella Iannuzzi and Tatiana Marchenko\*



1245

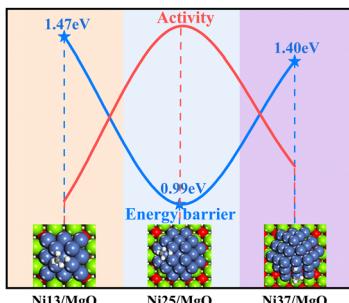
## Effect of the charge rate on the mechanical response of composite graphite electrodes: *in situ* experiment and mathematical analysis

Hainan Jiang, Yaolong He, Xiaolin Li, Zhiyao Jin, Huijie Yu\* and Dawei Li\*



## RESEARCH PAPERS

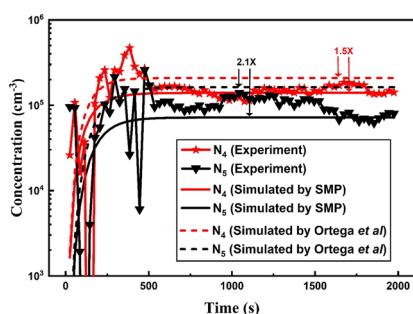
1255



### Unraveling the effect of particle size of active metals in Ni/MgO on methane activation and carbon growth mechanism

Shengzhuo Chen, Juntian Niu,\* Xianrong Zheng, Haiyu Liu, Yan Jin and Jingyu Ran

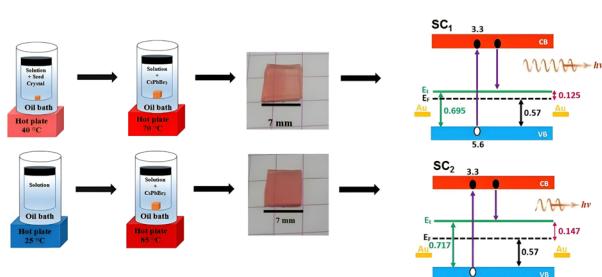
1267



### Growth mechanism prediction for nanoparticles via structure matching polymerization

Yi-Rong Liu\* and Yan Jiang

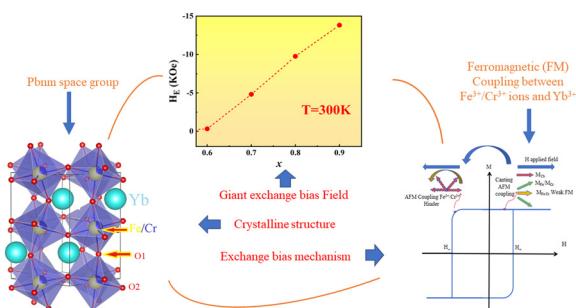
1274



### Growth methods' effect on the physical characteristics of CsPbBr₃ single crystal

Mohamed Ben Bechir\* and Faisal Alresheedi

1284



### Giant exchange bias field above room temperature in perovskite $\text{YbCr}_{1-x}\text{Fe}_x\text{O}_3$ ( $x = 0.6\text{--}0.9$ )

Kang Zhao, Dao Wang, Lei Wang\* and Sajjad Ur Rehman\*

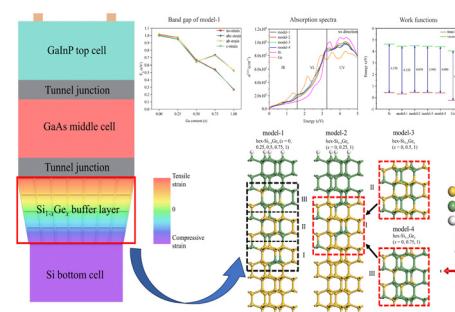


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1293

## A study on the $\text{Si}_{1-x}\text{Ge}_x$ gradual buffer layer of III–V/Si multi-junction solar cells based on first-principles calculations

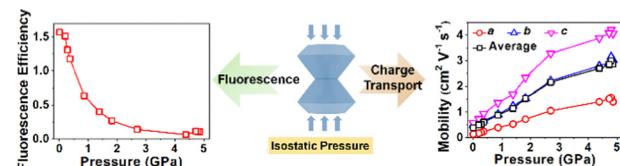
Qian Wang, Yu Zhuang,\* Abuduwayiti Aierken,\* Qiaogang Song, Qin Zhang, Youbo Dou, Qiuli Zhang and Shuyi Zhang



1303

## Pressure effects on both fluorescent emission and charge transport properties of organic semiconductors: a computational study

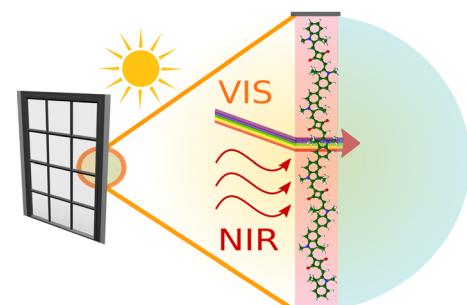
Yi Zeng, Wen Shi, Qian Peng, Yingli Niu, Zhiying Ma and Xiaoyan Zheng\*



1314

## Design of J-aggregates-like oligomers built from squaraine dyes exhibiting transparency in the visible regime and high fluorescence quantum yield in the NIR region

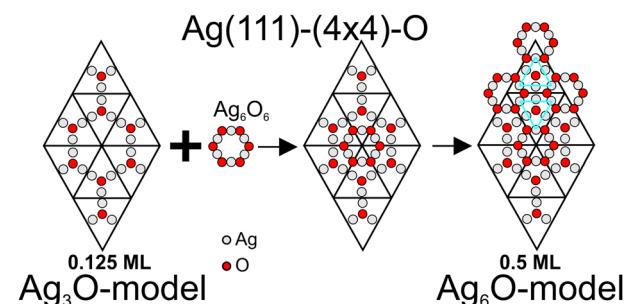
Margarita Bužančić Milosavljević and Vlasta Bonačić-Koutecký\*



1322

## New insights into the structure of the $\text{Ag}(111)-p(4 \times 4)-\text{O}$ phase: high-resolution STM and DFT study

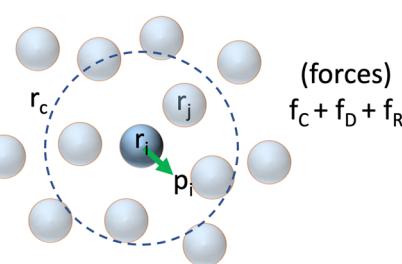
B. V. Andryushechkin,\* T. V. Pavlova and V. M. Shevlyuga



## RESEARCH PAPERS

1328

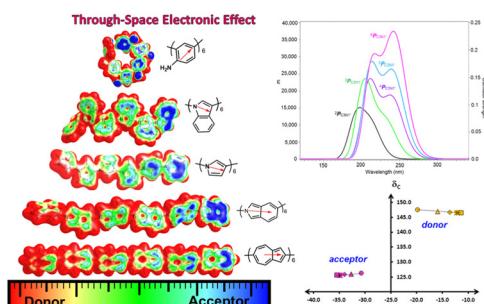
## Mechanical balance



## Green–Kubo expressions for transport coefficients from dissipative particle dynamics simulations revisited

D. C. Malaspina, M. Lísal, J. P. Larentzos, J. K. Brennan, A. D. Mackie and J. Bonet Avalos\*

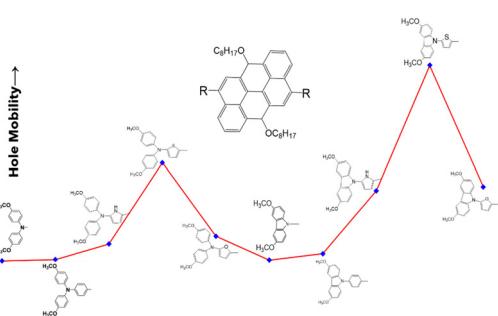
1340



## Utilization of the through-space effect to design donor–acceptor systems of pyrrole, indole, isoindole, azulene and aniline

Puthannur K. Anjalikrishna and Cherumuttathu H. Suresh\*

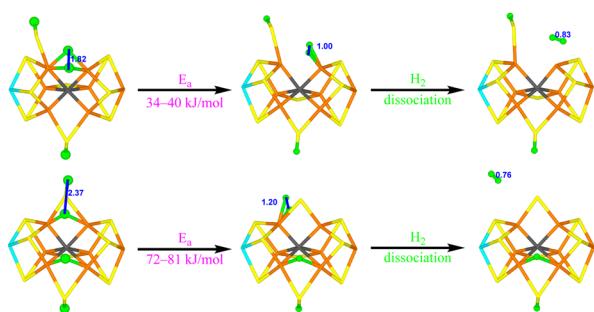
1352



## Effect of substituting donors on the hole mobility of hole transporting materials in perovskite solar cells: a DFT study

Md Al Mamunur Rashid, Sein Min, Sung Keon Namgoong and Keunhong Jeong\*

1364

H<sub>2</sub> formation from the E<sub>2</sub>–E<sub>4</sub> states of nitrogenase

Hao Jiang and Ulf Ryde\*

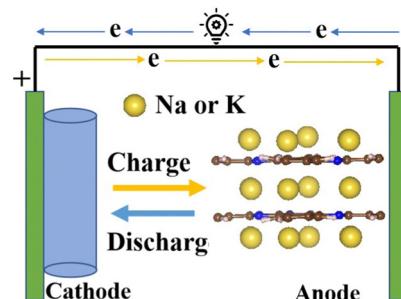


## RESEARCH PAPERS

1376

**First principles study of a triazine-based covalent organic framework as a high-capacity anode material for Na/K-ion batteries**

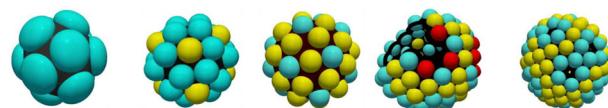
Sitong Liu, Bo Liu,\* Meidong Yu, Hanyu Gao, Haipeng Guo, Daguo Jiang, Shenbo Yang, Yufeng Wen\* and Yabei Wu



1385

**Breaking the size constraint for nano cages using annular patchy particles**

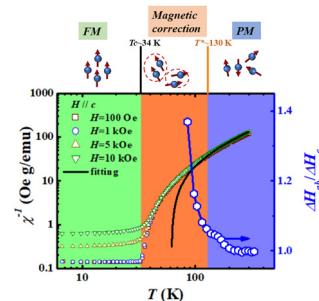
Vikki Anand Varma, Simmie Jaglan, Mohd Yasir Khan and Sujin B. Babu\*



1396

**Observation of the possible magnetic correction above the Curie temperature in  $\text{Cr}_2\text{Si}_2\text{Te}_6$  single crystals**

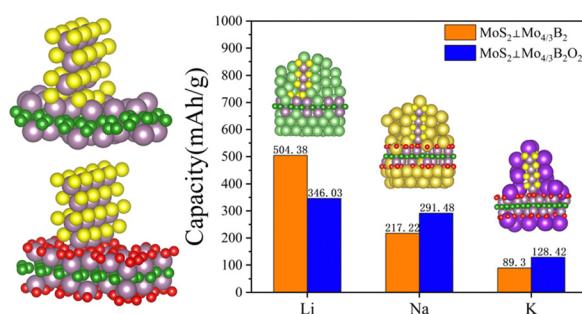
Yan Sun,\* Zhongzhu Jiang, Yang Li, Lanxin Liu, Hui Liang, Yiyuan Wang, Dandan Wu, Na Li, Ying Zhou, Qiuju Li, Xiaoyu Yue, Wei Tong, Xuan Luo, Jianghe Lan\* and Xuefeng Sun\*



1406

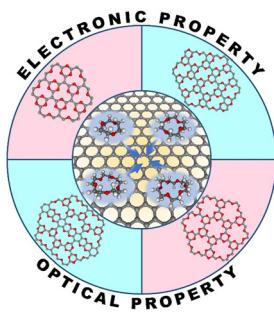
**Improved ion adsorption capacities and diffusion dynamics in surface anchored  $\text{MoS}_2 \perp \text{Mo}_{4/3}\text{B}_2$  and  $\text{MoS}_2 \perp \text{Mo}_{4/3}\text{B}_2\text{O}_2$  heterostructures as anodes for alkaline metal-ion batteries**

Zifeng Song, Haoliang Liu, Baiyi Chen, Qin Jiang, Fengxiang Sui, Kai Wu, Yonghong Cheng and Bing Xiao\*



## RESEARCH PAPERS

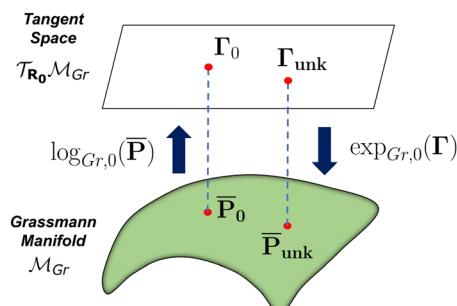
1428



**Dense arrangement of crown ethers in graphene: novel graphitic carbon oxides with enhanced optoelectronic properties**

Hongyan Li, Jiang Xiang, Liang Chen, Jing Xu\* and Wei Liu\*

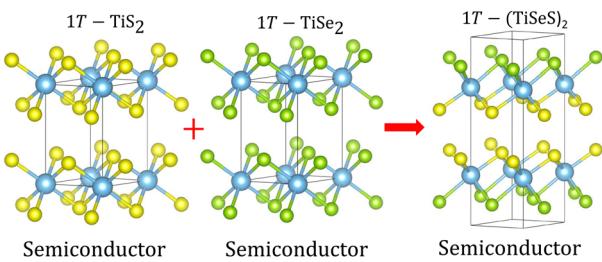
1436



**Mapping spin contamination-free potential energy surfaces using restricted open-shell methods with Grassmannians**

Jake A. Tan\* and Ka Un Lao\*

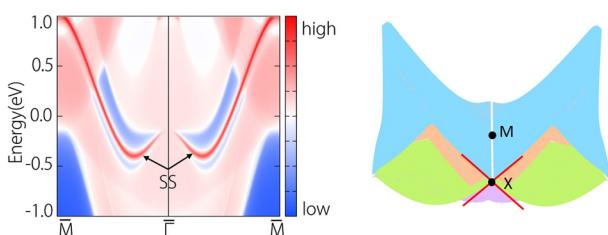
1443



**Janus layers and electronic structure of 1T-(TiSeS)<sub>2</sub>**

Yue Lou\* and Ping Lou\*

1454



**Coexistence of topological node surface and Dirac fermions in phonon-mediated superconductor YB<sub>2</sub>C<sub>2</sub>**

Siqi Wang, Mingmin Zhong,\* Haibo Liu and Meng Ju



## CORRECTION

1462

**Correction: Extracting accurate information from triplet–triplet annihilation upconversion data with a mass-conserving kinetic model**

Abhishek Kalpattu, Tristan Dilbeck, Kenneth Hanson and John T. Fourkas\*

