

# PCCP

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### Cover

See Tiia Jacklin, Perttu Lantto *et al.*, pp. 14759–14766. Image reproduced by permission of Tiia Jacklin from *Phys. Chem. Chem. Phys.*, 2025, 27, 14759.



### Inside cover

See Emiliano De Santis, Carl Coleman *et al.*, pp. 14767–14776. Image reproduced by permission of Erik G. Marklund from *Phys. Chem. Chem. Phys.*, 2025, 27, 14767.

## EDITORIAL

14702

### PCCP 25th anniversary collection

Bee Hockin\* and Anouk M. Rijs

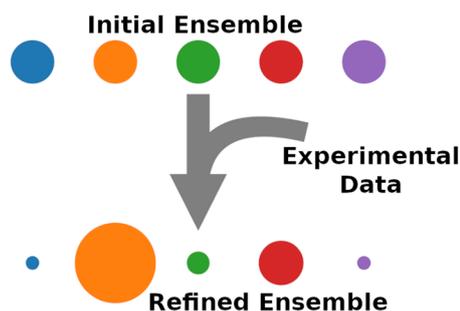


## PERSPECTIVES

14704

### Combining simulations and experiments – a perspective on maximum entropy methods

Johannes Stöckelmaier and Chris Oostenbrink\*



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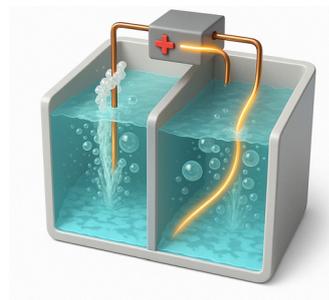
Fundamental questions  
Elemental answers



## PERSPECTIVES

14718

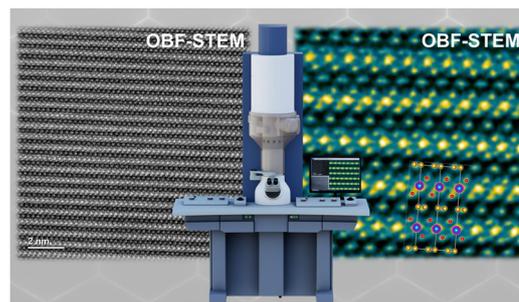
## New perspectives addressing application challenges in concentration cells

Zeshuo Meng,\* Runlin Zhang, Haoteng Sun,\*  
Jingchen Zhang, Xiliang Gong and Zhengyan Du\*

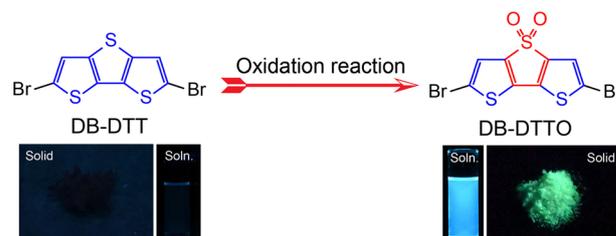
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14729

## Probing the atomic arrangement of honeycomb layered oxides via optimum bright-field scanning transmission electron microscopy (OBF-STEM)

Titus Masese,\* Godwill Mbiti Kanyolo,\*  
Yoshinobu Miyazaki, Kimiya Sukegawa and  
Tomohiro Saito

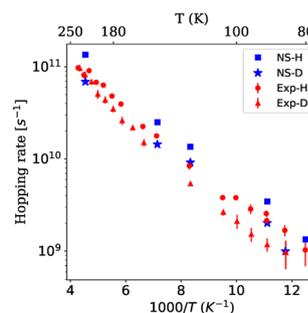
14733

Oxidation reduces spin-orbital coupling to achieve robust fluorescence emission in halogen-substituted dithieno[3,2-*b*:2',3'-*d*]thiopheneHuimin Liu, Zeyan Zhuang, Yawen Hou, Yujiao Zhu,  
Ruofeng Xu, Bin Chen,\* Rong Hu\* and Zujin Zhao\*

14739

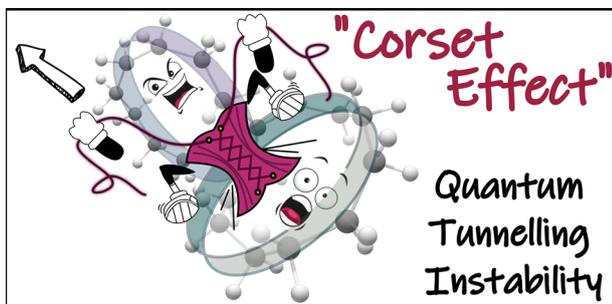
## Incoherent tunneling surface diffusion

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



## COMMUNICATIONS

14744

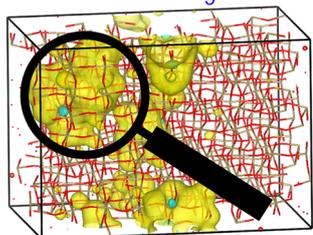


How small can a catenane be, if we consider quantum tunnelling?

Sindy Julieth Rodriguez-Sotelo,  
Juan Julian Santoyo-Flores and Sebastian Kozuch\*

14748

How do polarons form in  $\text{NaTaO}_3$ ?

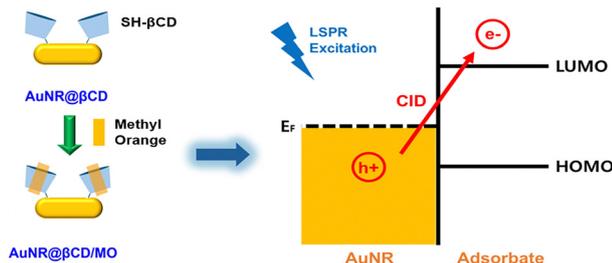


Quantum-chemical molecular dynamics study of polaron formation in perovskite  $\text{NaTaO}_3$  as a water-splitting photocatalyst

Hiroki Uratani\* and Hiroshi Onishi

14754

CID Using Host-Guest Interactions on AuNR

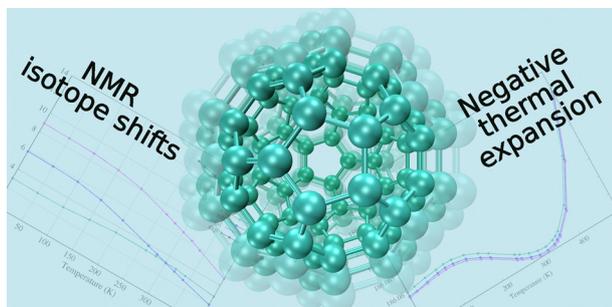


Thiolated  $\beta$ -cyclodextrin-based host-guest interactions: investigating and tuning chemical interface damping in single gold nanorods

Minji Kim, Yola Yolanda Alizar,  
Rafifah Hana Raihana Syam and Ji Won Ha\*

## RESEARCH PAPERS

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Quantum-mechanical treatment of thermal effects on the structure and  $^{13}\text{C}$  NMR shielding of buckminsterfullerene  $\text{C}_{60}$

Tiia Jacklin,\* Petr Štěpánek and Perttu Lantto\*

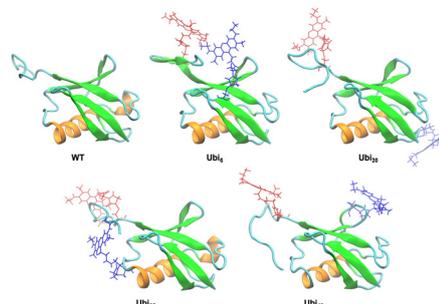


## RESEARCH PAPERS

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### Structural stability of chromophore-grafted Ubiquitin mutants in vacuum

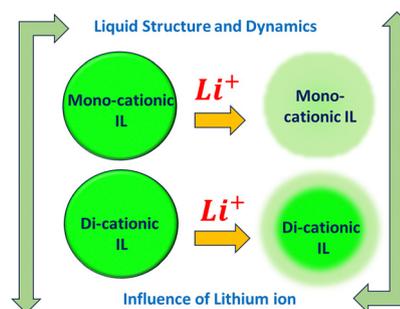
Emiliano De Santis,\* Thomas Mandl, Jocky C. K. Kung, Khon Huynh, Steven Daly, Lorenza A. D'Alessandro, Luke MacAleese, Charlotte Uetrecht, Erik G. Marklund and Carl Caleman\*



14777

### Probing lithium-ion induced micro-environment changes in pyrrolidinium-based mono-cationic and di-cationic ionic liquids

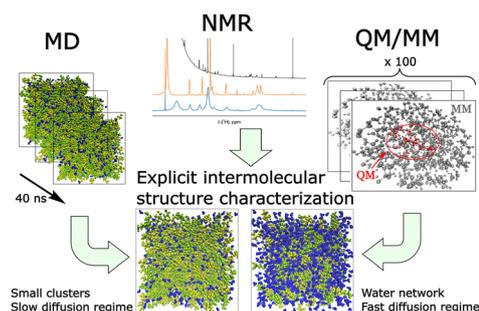
Amita Mahapatra, Umesh D. Chowdhury, Subahakanta Parida, Sahadev Barik, Joyoti Ghosh, B. L. Bhargava and Moley Sarkar\*



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### Intermolecular organization in aqueous mixtures of choline lysinate studied *via* NMR and molecular dynamics/quantum mechanics

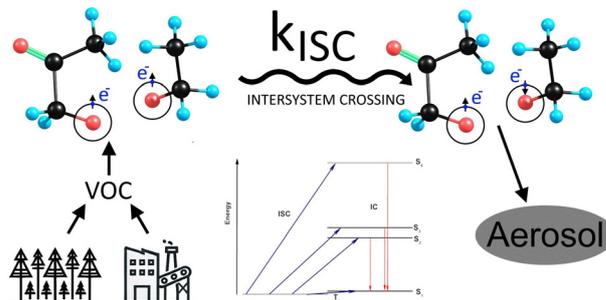
Einaras Sipavičius, Lukas Mikalauskas, Vytautas Klimavicius and Kęstutis Aidas\*



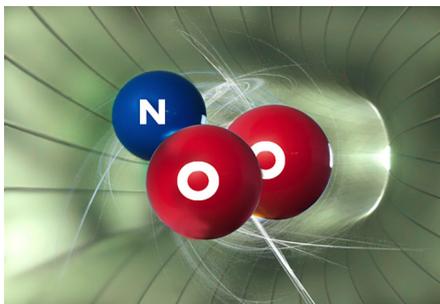
14804

### Predicting intersystem crossing rate constants of alkoxy-radical pairs with structure-based descriptors and machine learning

Rashid R. Valiev,\* Rinat T. Nasibullin, Hilda Sandström, Patrick Rinke, Kai Puolamäki and Theo Kurten\*



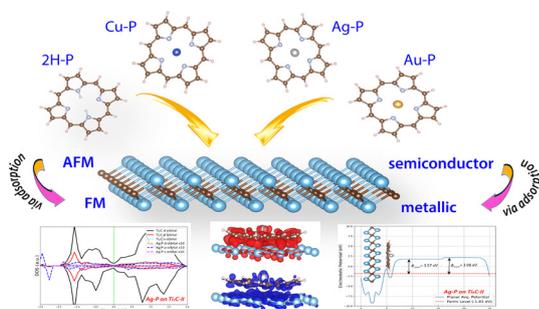
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### Exploring quantum tunneling in heavy atom reactions using a rigorous theoretical approach to the dynamics: formation of NO + O from the N + O<sub>2</sub> atmospheric reaction

Fabrizio Esposito, Pablo Gamallo, Miguel González\* and Carlo Petrongolo

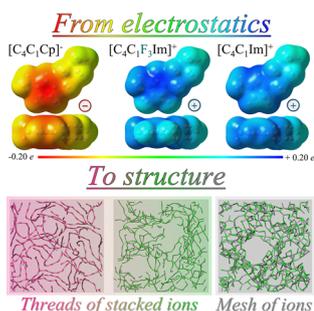
14829



### Magnetic transition and work function modulation of Ti<sub>2</sub>C MXene *via* porphine adsorption

Pınar Kaya, Çağıl Kaderoğlu,\* Ethem Aktürk and Handan Arkin

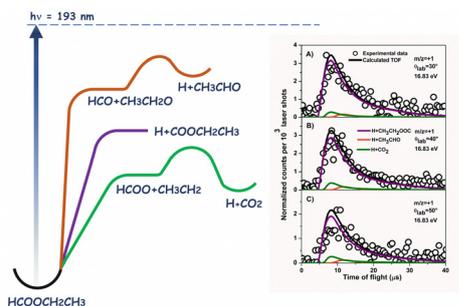
14841



### Rational design of halo-imidazolium-based ionic liquids: tailoring the charge distribution to mimic the structure of real charge inverted analogues

Lois Morandeira,\* Tiago F. C. Cruz, Pedro T. Gomes, José N. Canongia Lopes and Karina Shimizu\*

14851



### Photodissociation dynamics of ethyl formate at 193 nm-based synchrotron radiation and *ab initio* calculations: hydrogen elimination and secondary dissociations

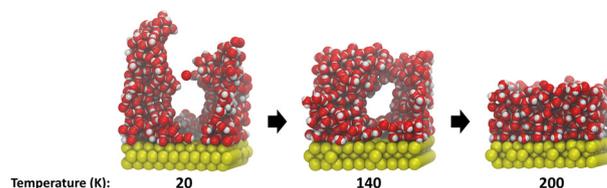
Orlando Dominguez-Flores, Rodrigo Navarro-Severiano, David Ochoa-Resendiz, Oscar Quiroz-Cardoso, Annia Rodriguez-Hernandez, Jesus Porcayo-Calderon, Francisco Javier Hernandez-Campos, Shih-Huang Lee, Ramon Hernandez-Lamonedada and Alfredo Quinto-Hernandez\*



14864

### A molecular dynamics study of the effect of annealing temperature on the structure of ASW

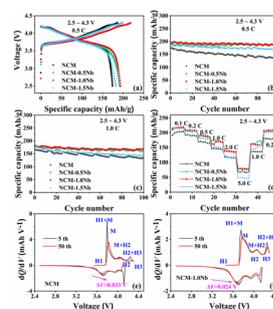
Zachary Amato,\* Thomas F. Headen, Pierre Ghesquière and Helen J. Fraser



14884

### Enhancement of the cycling stability of the nickel-rich cathode material $\text{LiNi}_{0.9}\text{Co}_{0.01}\text{Mn}_{0.09}\text{O}_2$ via $\text{Nb}^{5+}$ doping

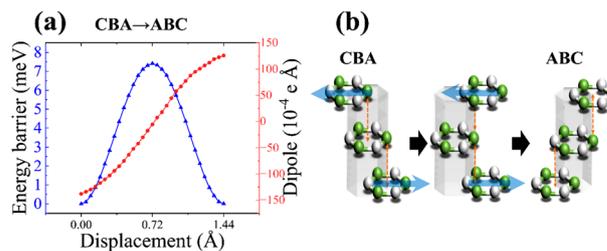
Jiatai Wang,\* Chao Fan, Yuanyuan Li, Yan Tan, Xuchao Zhang, Jiting Li, Hongyun Liu, Xiaohong Ma, Changjuan Deng and Jian Li



14896

### Sliding ferroelectricity of multilayer h-BN

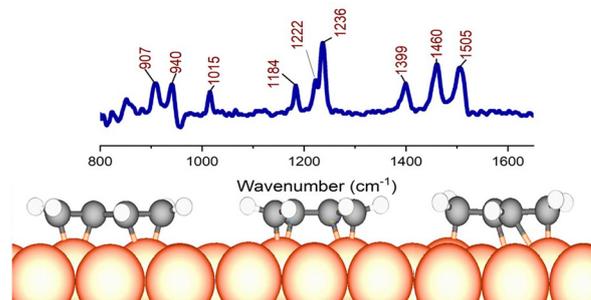
Zijun Li, Le Fang, Hui Zhang,\* Wei Wu\* and Wei Ren\*



14906

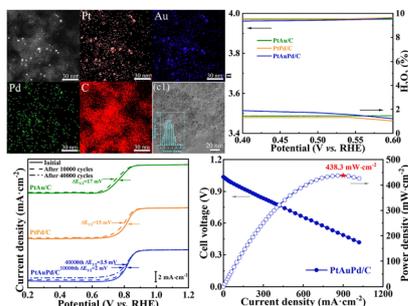
### Structure of chemisorbed 1,3-butadiene on the $\text{Cu}(111)$ surface

Mohammad Rahat Hossain, Ahmad Arshadi, Ye Xu\* and Michael Trenary\*



## RESEARCH PAPERS

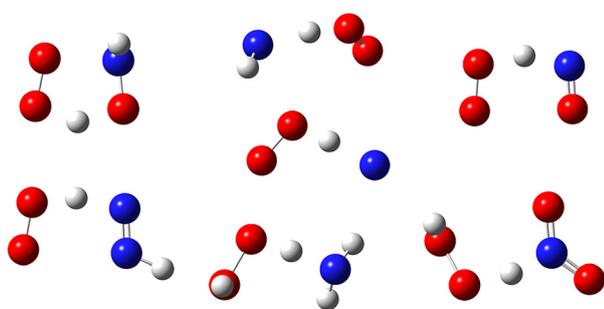
14914



### Electrocatalytic activity of PtAuPd/C nano multi-principal element alloy catalyst towards oxygen reduction reaction

Hui Li, Zhiwei Zhang, Lianke Zhang, Hualiang Ni, Haiying Qin,\* Jing Zhang,\* Hongzhong Chi and Junjing He

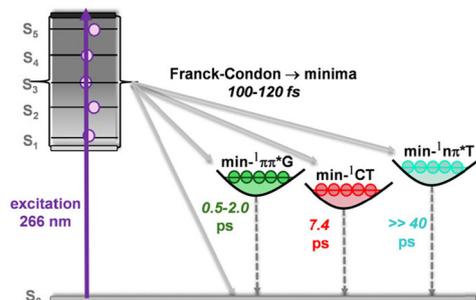
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### Overlooked hydroperoxyl radical reactions in ammonia oxidation under combustion conditions

Kfir Kaplan, Michal Keslin and Alon Grinberg Dana\*

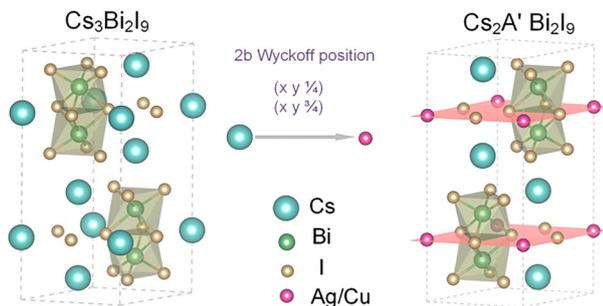
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### Ultrafast dynamics of the UV-induced electronic relaxation in DNA guanine–thymine dinucleotides: from the Franck–Condon states to the minima of the potential energy surfaces

Vasilis Petropoulos, Lara Martinez-Fernandez,\* Lorenzo Ubaldi, Margherita Maiuri, Giulio Cerullo,\* Evangelos Balanikas and Dimitra Markovitsi\*

14948



### Enhanced charge transport in A-site ordered perovskite derivatives $A_2A'Bi_2I_9$ ( $A = Cs$ ; $A' = Ag, Cu$ ): a first-principles study

Shuhan Li, Siyu Song, Peng Lv,\* Shihao Wang, Jiawang Hong and Gang Tang\*

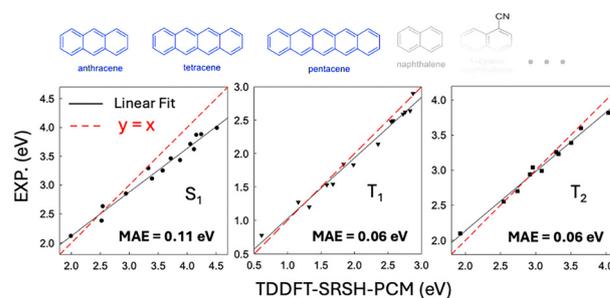


## RESEARCH PAPERS

14957

### Accurate prediction of the energies of the lowest excited states, $S_1$ , $T_1$ , and $T_2$ , of chromophores for improving solar cell applications

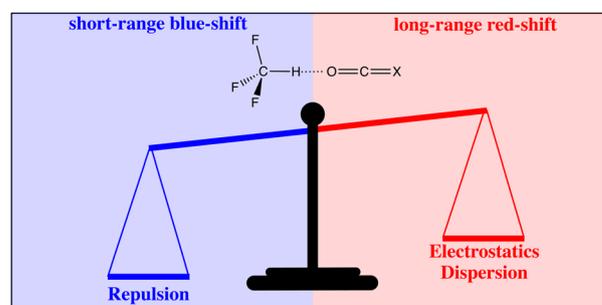
Muhammet Erkan Köse, Roshan Khatri and Barry D. Dunietz\*



14966

### Tetrel, nonconventional hydrogen bonds, and noticeable role of dispersion in complexes of fluoroform and carbon dichalcogenides

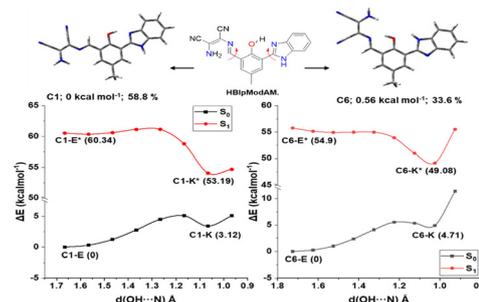
Thanh-Nam Huynh, Nguyen Thi Minh Nguyet, Bui Duc Ai and Nguyen Tien Trung\*



14976

### Excited-state relaxation mechanisms of Janus-type proton in benzimidazole-conjugated aminomaleonitrile: single or double proton transfer?

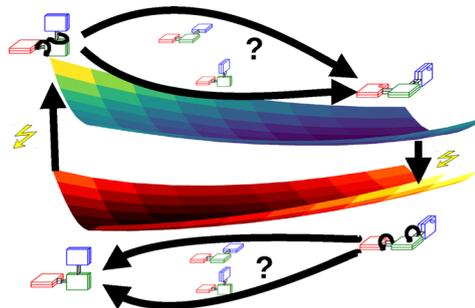
Sonika, Sukhvinder Dhiman, Ashutosh Sharan Singh, Vijay Luxami and Gulshan Kumar\*



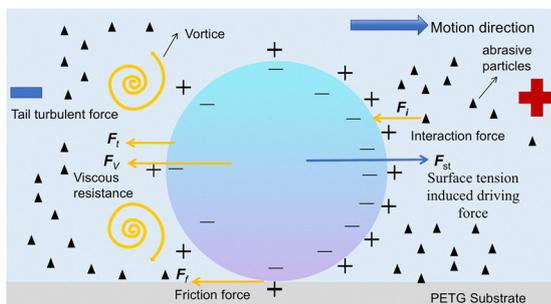
14985

### Surface hopping simulations reveal deactivation pathways of a charge transfer system with planarizing and twisting motion

Julia Haberhauer,\* Sebastian Mai, Leticia González and Christof Hättig\*



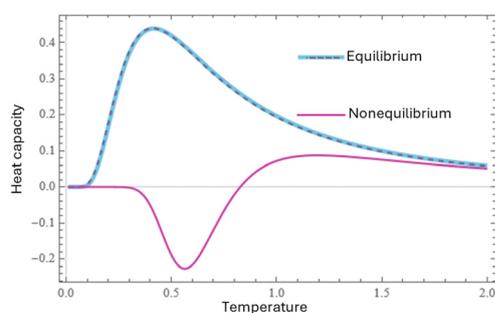
14999



## Dynamic behaviour of electrically driven liquid metal droplets in abrasive particle suspensions

Baoqi Feng, Kaixiang Li, Yapeng Ma and Lei Zhang\*

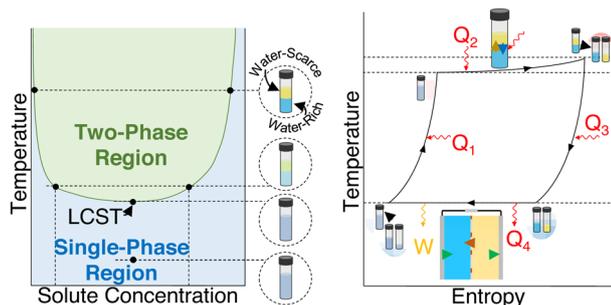
15009



## Negative specific heats: where Clausius and Boltzmann entropies separate

Lander Bogers, Faezeh Khodabandehlou and Christian Maes

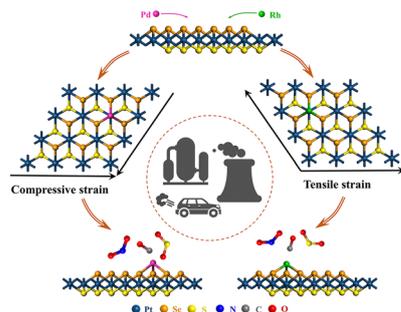
15024



## Thermodynamic properties of lower critical solution temperature (LCST) mixtures for application in energy–water systems

Jordan D. Kocher, Ahmed Mahfouz, Jesse G. McDaniel and Akanksha K. Menon\*

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## Synergistic enhancement of gas sensor performance in Janus PtSse monolayer via Pd/Rh decoration and strain engineering: a first-principles investigation

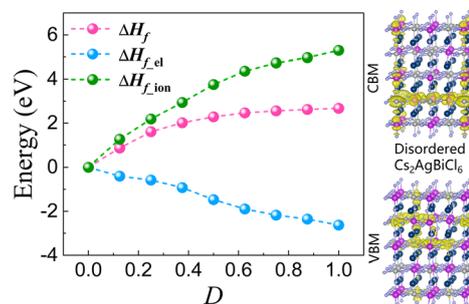
Xiao Wang, Yang Li,\* Xinglian Yang, Rongji Zhang, Rongbiao Xiang, Junyu Chen, Zhilong Peng, Qiang Fu\* and Jiamu Cao\*



15049

## Elucidating the role of lone-pair $ns^2$ electrons on B-site cation disordering in double halide perovskites $\text{Cs}_2\text{AgBiCl}_6$ and $\text{Cs}_2\text{AgInCl}_6$

Jingting Wei, Jiayin Wu, Yibin Yang, Le Huang\* and Bin Li\*



15055

## Modeling the Monty Hall decision problem with reaction kinetics

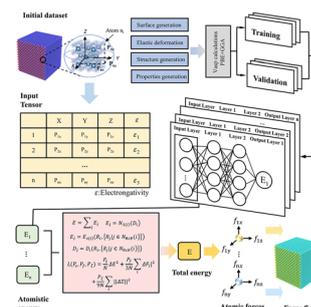
Oliver Steinbock\* and Wen Zhu\*



15062

## Machine learning molecular dynamics reveals atomistic mechanisms of ion beam damage in calcium fluoride

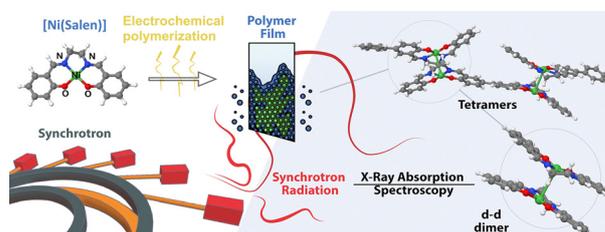
Zixuan Chen, Jixiang Ding, Shayu Song, Rongtao Shen, Jianguo Zhang,\* Junfeng Xiao and Jianfeng Xu



15080

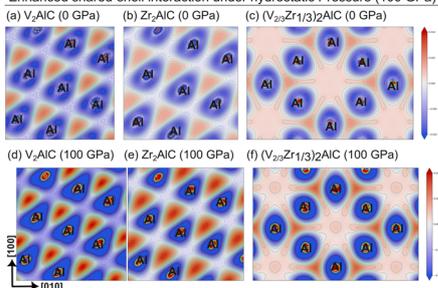
## The structure of the $\text{NiO}_2\text{N}_2$ coordination center in the $[\text{Ni}(\text{Salen})]$ complex and its polymer: a comparative study by X-ray absorption spectroscopy and quantum-chemical calculations

Petr M. Korusenko,\* Olga V. Petrova, Anatoliy A. Vereshchagin, Oleg V. Levin, Evgeny V. Khramov, Ratibor G. Chumakov, Mikhail A. Soldatov, Konstantin P. Katin, Alexander S. Konev and Alexander S. Vinogradov



15099

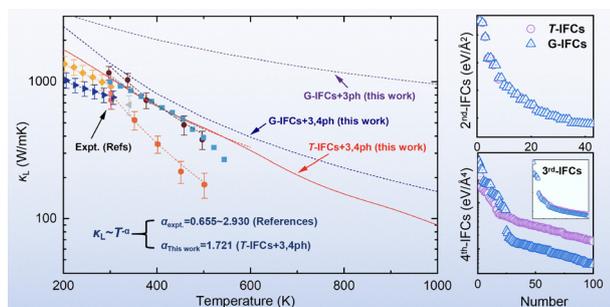
Enhanced shared-shell interaction under hydrostatic Pressure (100 GPa)



**First-principles study of the structural, electronic, elastic, and high-pressure properties of the  $(V_{2/3}Zr_{1/3})_2AlC$  i-MAX phase and  $M_2AlC$  ( $M = V, Zr$ ) MAX phases**

Rashid Khan, Qingmin Zhang and Shafqat Hussain Shah\*

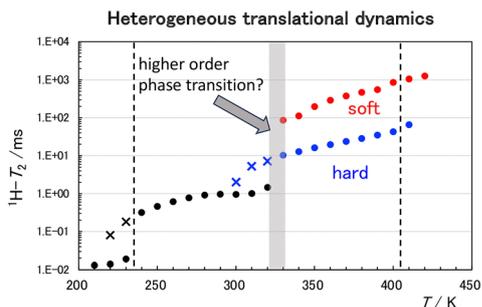
15119



**Accurately predicting the thermal conductivity of boron arsenide considering the temperature-induced phonon anharmonic renormalization: a critical revisit**

Yongjun Wu, Yan Zhang and Zhen Tong\*

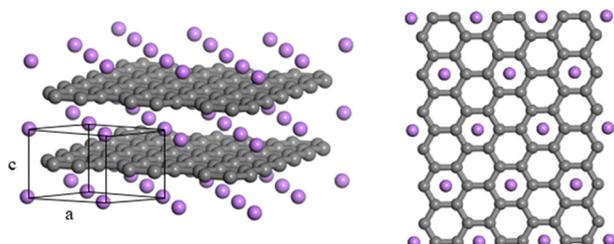
15126



**Nuclear magnetic resonance study of the relationship between phase behaviour and reorientational and translational dynamics in  $N,N$ -diethylpyrrolidinium bis(fluorosulfonyl)amide with a plastic crystal phase**

Keiko Nishikawa,\* Kozo Fujii and Masahiro Yoshizawa-Fujita\*

15137



**Tuning the thermal conductivity of lithium intercalated graphite through temperature, strain, and interlayer twist angles**

Kaiyu Yang, Na Di, Yu Liu\* and Guangzhao Qin

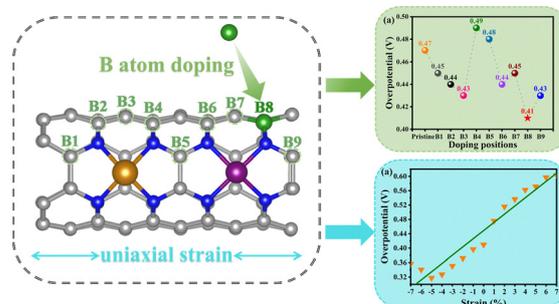


## RESEARCH PAPERS

15148

### Improving the activity of the oxygen evolution reaction on $\text{TiN}_4\text{-CoN}_4$ embedded carbon nanotubes *via* boron atom doping and applying uniaxial strain

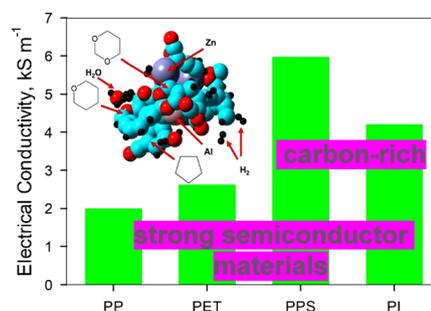
Xing-Chen Ding, Bao-Tong Cong, Wen-Hui Zhao, Zi-Qiang Deng, Long-Hui Li, Shi-Yao Liu, Zhen-Kun Tang\* and Hui Zhang\*



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### Insulator and electrode materials marginally influence carbonized layer conductivity in metalized-film capacitors

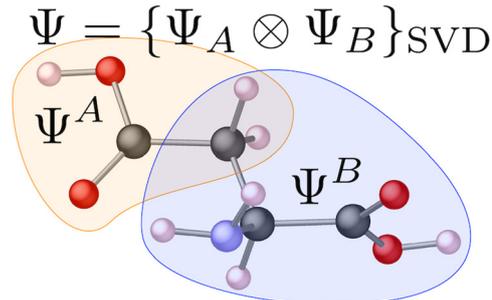
Vitaly V. Chaban\* and Nadezhda A. Andreeva



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### The overlapping fragment approach for non-orthogonal configuration interaction with fragments

C. Sousa, X. Dong, R. Broer, T. P. Straatsma and C. de Graaf\*



15176

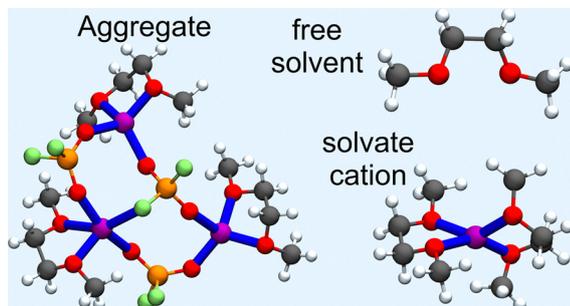
### Insight into the characteristics of carbonized ZIF-8 for the separation of Kr and Xe

Peng Lin, Genggeng Dai, Xiaohua Liu, Yingzhe Du, Zhiguo Li, Duo Zhang, Wentao Zhou\* and Fangbo Zhao\*



## RESEARCH PAPERS

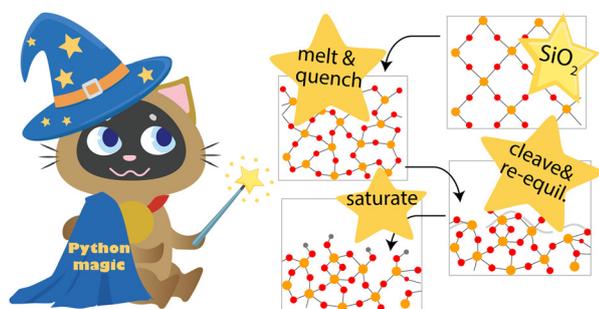
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### Discrepant lithium transference numbers due to heterogeneous speciation

Frederik Philippi,\* Yuna Matsuyama, Simon Buying, Taku Sudoh, Keisuke Shigenobu, Wataru Shinoda, Monika Schönhoff, Masayoshi Watanabe and Kazuhide Ueno

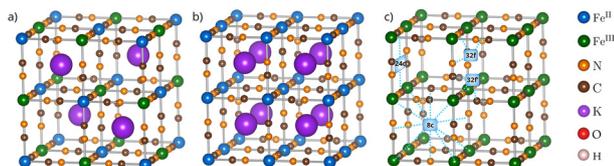
15196



### Ground-up generation of periodic slab models of dehydroxylated amorphous silica of varying roughness

Mas P. Klein, Evgeny A. Pidko and Alexander A. Kolganov\*

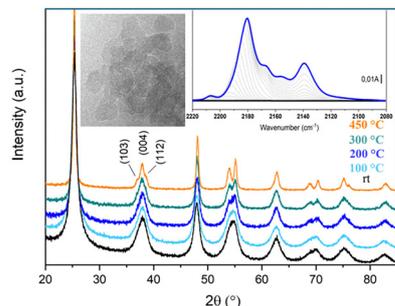
15204



### Dependence of the crystal structure of Prussian blue on the occupation of interstitial sites

Maria Vitória Cavalheiro Issler, Cristiano Vicente, Iuri Stefani Brandt, Bruna Fernanda Baggio, Ricardo Faccio, Milton Andre Tumelero\* and André Avelino Pasa\*

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### Effect of thermal treatments on high surface area anatase TiO<sub>2</sub>

Chiara Nannuzzi,\* Ton V. W. Janssens and Gloria Berlier\*

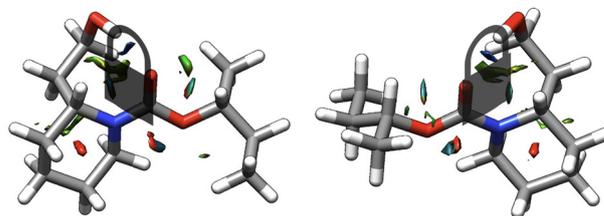


## RESEARCH PAPERS

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**Hydrogen-bond-assisted conformational selection of picaridin in the gas phase**

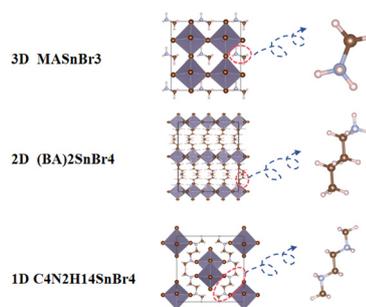
Otger Crehuet, Andrea Vázquez, Francisco J. Basterretxea, Pablo Pinacho\* and Emilio J. Cocinero\*



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**Differences and regulation of self-trapped luminescence in one-dimensional Pb-based and Sn-based perovskites**

Jun Luo, Zhi-Ming Luo, Biao Liu, Jun-Liang Yang and Meng-Qiu Cai\*



## RETRACTIONS

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**Retraction: Atomic diffusion of sulfate and chloride ions in the nanometer cavity of C-S-H/Nanoclay**

Ali Dalvand, Seyed Amir Hossein Hashemi, Reza Farokhzad and Ali Delnavaz

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**Retraction: Atomic Interactions Solidified Through the Introduction of Cellulose Nanocrystals to Cementitious Matrix: a Theoretical Study at the Molecular Level**

Seyyed Mohammad Amin Fattahi, Seyed Amir Hossein Hashemi, Reza Farokhzad and Ali Delnavaz

