Open Access Article. Published on 17 July 2025. Downloaded on 12/12/2025 6:01:18 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

PCCP

Physical Chemistry Chemical Physics – An international journal

rsc.li/pccp

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 27(28) 14685–15240 (2025)

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 Caleman *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**

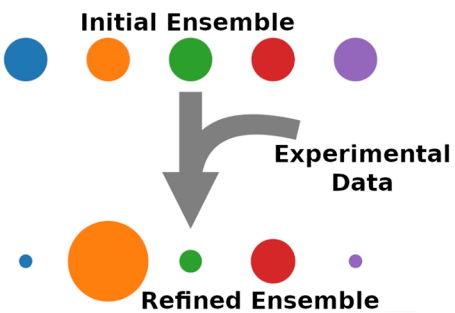
Bee Hockin* and Anouk M. Rijs

PERSPECTIVES

14704

Combining simulations and experiments – a perspective on maximum entropy methods

Johannes Stöckelmaier and Chris Oostenbrink*



View Article Online

ROYAL SOCIETY OF CHEMISTRY

Open Access Article. Published on 17 July 2025. Downloaded on 12/12/2025 6:01:18 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

EES Catalysis

GOLD OPEN ACCESS

Exceptional research on energy and environmental catalysis

Open to everyone. Impactful for all

rsc.li/EESCatalysis

Fundamental questions
Elemental answers

Registered charity number: 207890

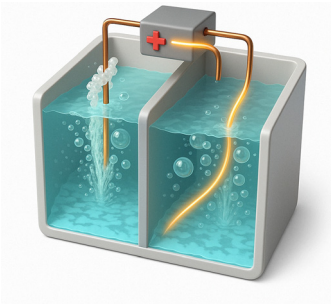
Open Access Article. Published on 17 July 2025. Downloaded on 12/12/2025 6:01:18 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

PERSPECTIVES

14718

New perspectives addressing application challenges in concentration cells

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

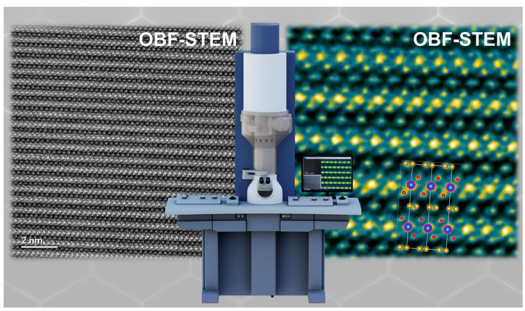


COMMUNICATIONS

14729

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

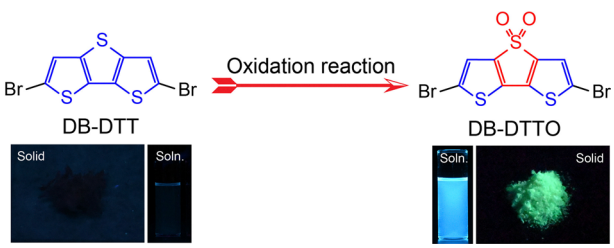
Titus Masese,* Godwill Mbiti Kanyolo,* Yoshinobu Miyazaki, Kimiya Sukegawa and Tomohiro Saito



14733

Oxidation reduces spin-orbital coupling to achieve robust fluorescence emission in halogen-substituted dithieno[3,2-*b*:2′,3′-*d*]thiophene

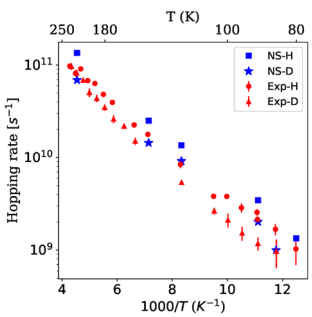
Huimin Liu, Zeyan Zhuang, Yawen Hou, Yujiao Zhu, Ruofeng Xu, Bin Chen,* Rong Hu* and Zujin Zhao*



14739

Incoherent tunneling surface diffusion

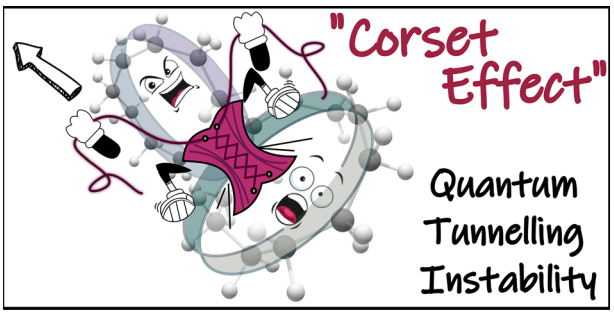
E. E. Torres-Miyares* and S. Miret-Artés



Open Access Article. Published on 17 July 2025. Downloaded on 12/12/2025 6:01:18 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

COMMUNICATIONS

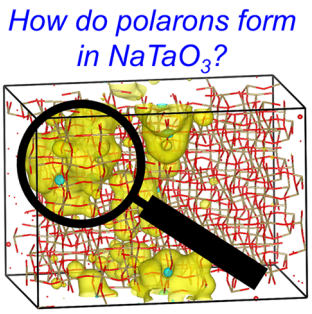
14744



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

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

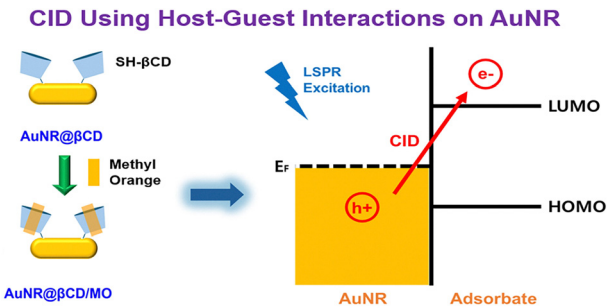
14748



Quantum-chemical molecular dynamics study of polaron formation in perovskite $NaTaO_3$ as a water-splitting photocatalyst

Hiroki Uratani* and Hiroshi Onishi

14754

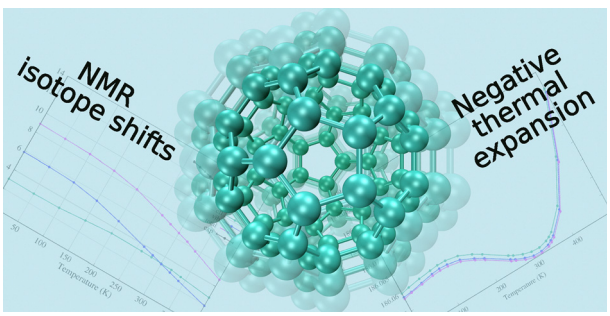


Thiolated β-cyclodextrin-based host–guest interactions: investigating and tuning chemical interface damping in single gold nanorods

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

RESEARCH PAPERS

14759



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

Tiia Jacklin,* Petr Štěpánek and Perttu Lantto*

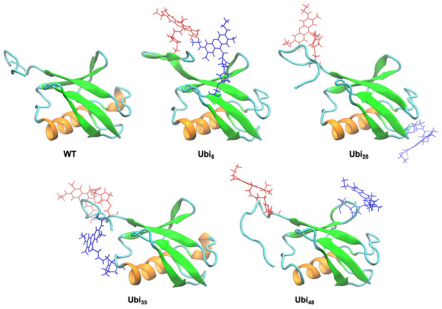
This journal is © the Owner Societies 2025

Open Access Article. Published on 17 July 2025. Downloaded on 12/12/2025 6:01:18 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

14767

Structural stability of chromophore-grafted Ubiquitin mutants in vacuum

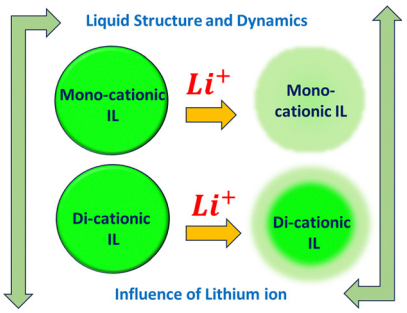
Emiliano De Santis,* Thomas Mandl, Jocky C. K. Kung, Khon Huynh, Steven Daly, Lorenza A. D'Alessandro, Luke MacAleese, Charlotte Uetrecht, Erik G. Marklund and Carl Caleman*



14777

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

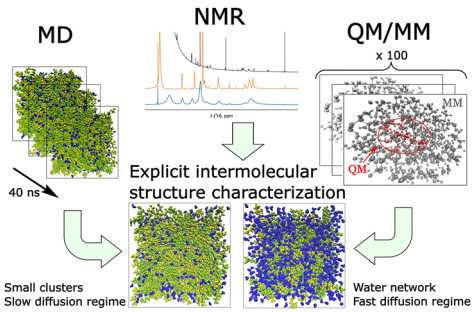
Amita Mahapatra, Unmesh D. Chowdhury, Subahakanta Parida, Sahadev Barik, Joyoti Ghosh, B. L. Bhargava and Moloy Sarkar*



14790

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

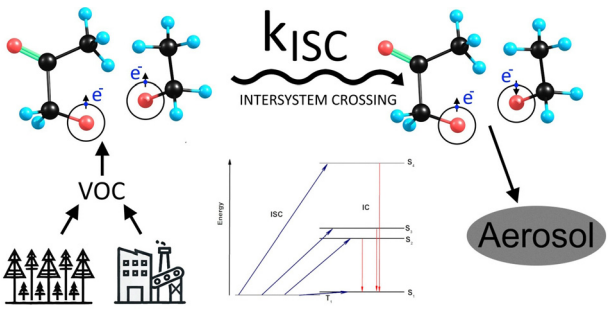
Einaras Sipavičius, Lukas Mikalauskas, Vytautas Klimavicius and Kęstutis Aidas*



14804

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

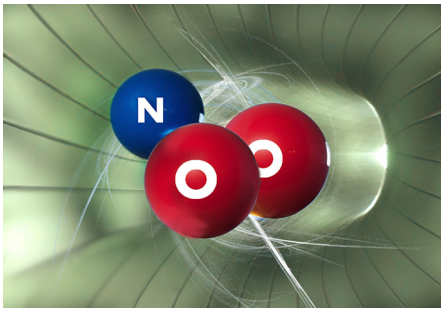
Rashid R. Valiev,* Rinat T. Nasibullin, Hilda Sandström, Patrick Rinke, Kai Puolamäki and Theo Kurten*



Open Access Article. Published on 17 July 2025. Downloaded on 12/12/2025 6:01:18 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

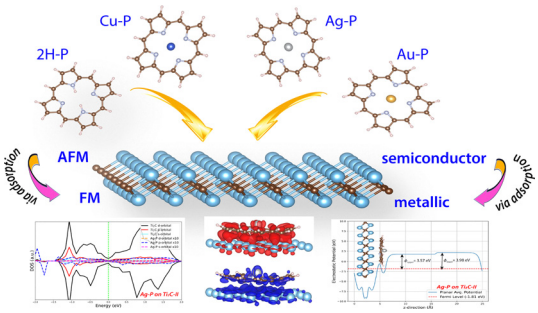
14815



Exploring quantum tunneling in heavy atom reactions using a rigorous theoretical approach to the dynamics: formation of NO + O from the N + O_2 atmospheric reaction

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

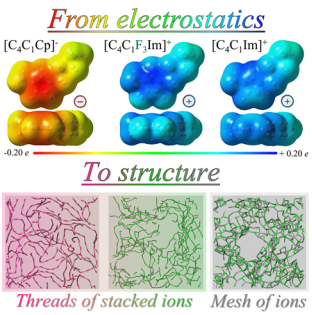
14829



Magnetic transition and work function modulation of Ti_2C MXene *via* porphine adsorption

Pınar Kaya, Çağıl Kaderoğlu,* Ethem Aktürk and Handan Arkın

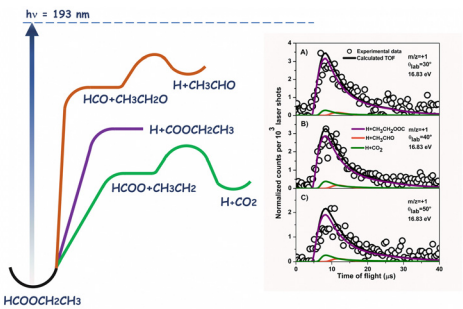
14841



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-Lamoneda and Alfredo Quinto-Hernandez*

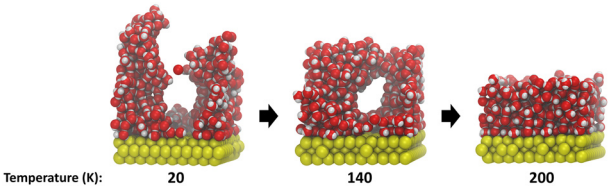
This journal is © the Owner Societies 2025

Open Access Article. Published on 17 July 2025. Downloaded on 12/12/2025 6:01:18 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

14864

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

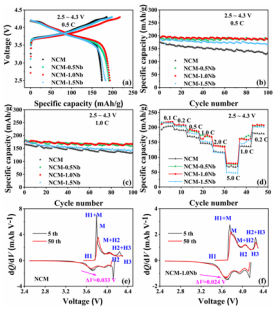
Zachary Amato,* Thomas F. Headen, Pierre Ghesquière and Helen J. Fraser



14884

Enhancement of the cycling stability of the nickel-rich cathode material $LiNi_{0.9}Co_{0.01}Mn_{0.09}O_2$ *via* Nb^{5+} doping

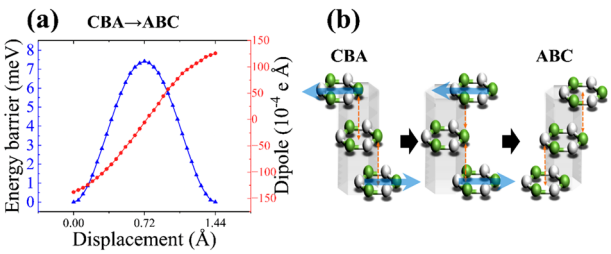
Jiatai Wang,* Chao Fan, Yuanyuan Li, Yan Tan, Xuchao Zhang, Jiting Li, Hongyun Liu, Xiaohong Ma, Changjuan Deng and Jian Li



14896

Sliding ferroelectricity of multilayer h-BN

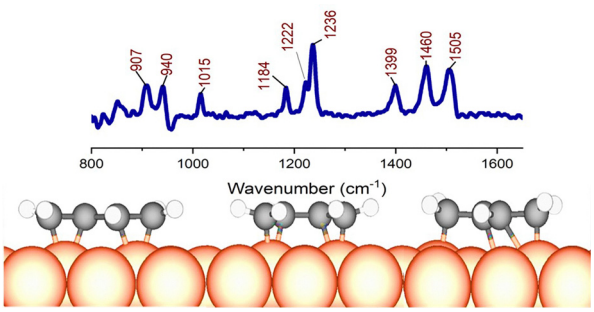
Zijun Li, Le Fang, Hui Zhang,* Wei Wu* and Wei Ren*



14906

Structure of chemisorbed 1,3-butadiene on the Cu(111) surface

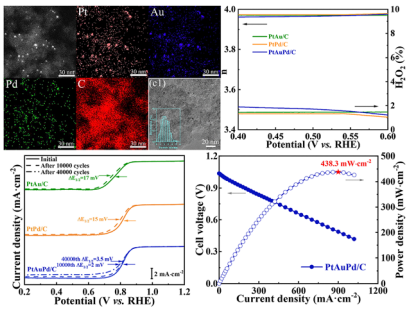
Mohammad Rahat Hossain, Ahmad Arshadi, Ye Xu* and Michael Trenary*



Open Access Article. Published on 17 July 2025. Downloaded on 12/12/2025 6:01:18 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

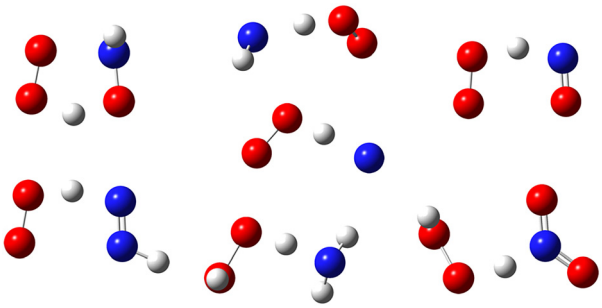
14914



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

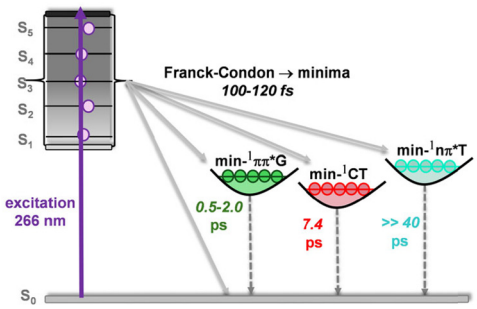
14924



Overlooked hydroperoxyl radical reactions in ammonia oxidation under combustion conditions

Kfir Kaplan, Michal Keslin and Alon Grinberg Dana*

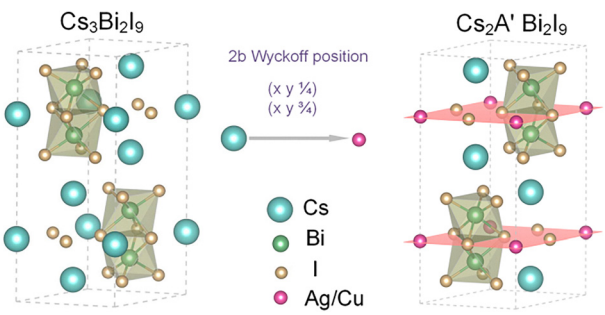
14936



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 Uboldi, 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*

This journal is © the Owner Societies 2025

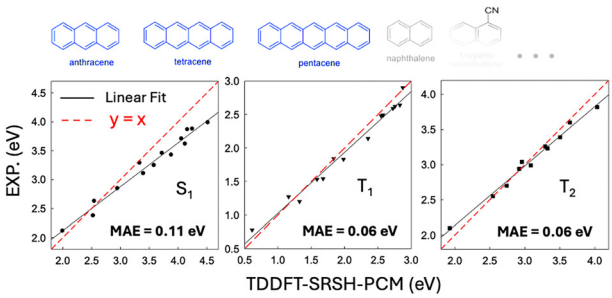
Open Access Article. Published on 17 July 2025. Downloaded on 12/12/2025 6:01:18 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

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

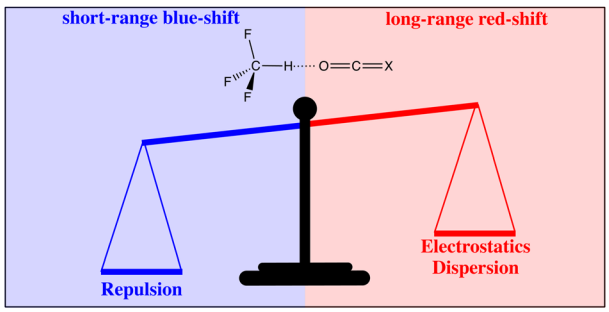
Muhammet Erkan Köse, Roshan Khatri and Barry D. Dunietz*



14966

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

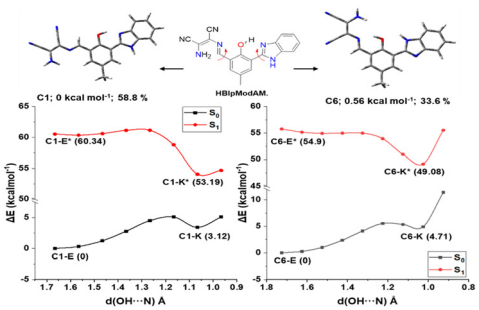
Thanh-Nam Huynh, Nguyen Thi Minh Nguyet, Bui Duc Ai and Nguyen Tien Trung*



14976

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

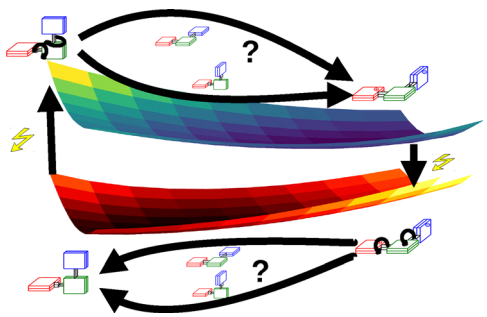
Sonika, Sukhvinder Dhiman, Ashutosh Sharan Singh, Vijay Luxami and Gulshan Kumar*



14985

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

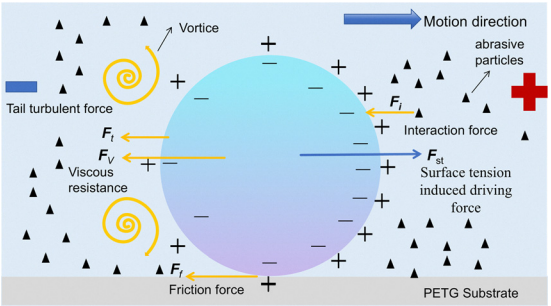
Julia Haberhauer,* Sebastian Mai, Leticia González and Christof Hättig*



Open Access Article. Published on 17 July 2025. Downloaded on 12/12/2025 6:01:18 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

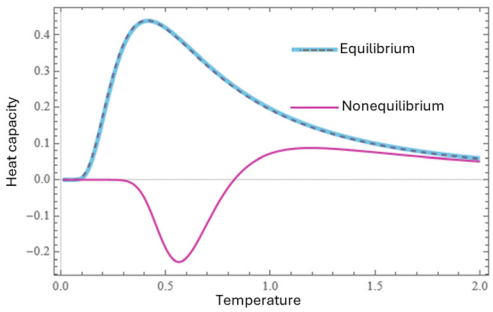
14999



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

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

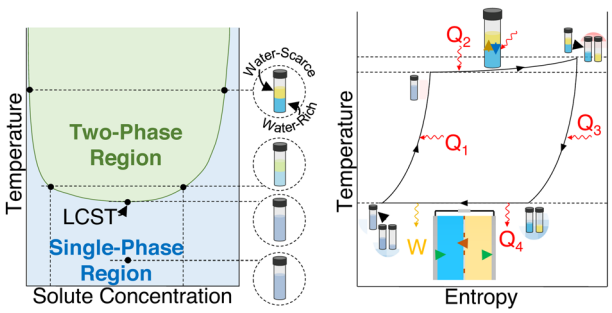
15009



Negative specific heats: where Clausius and Boltzmann entropies separate

Lander Bogers, Faezeh Khodabandehlou and Christian Maes

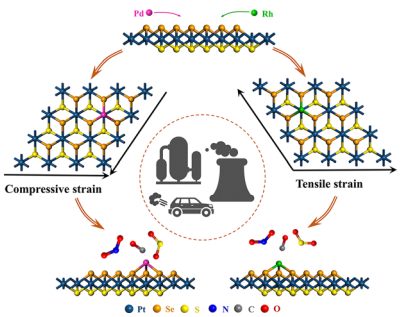
15024



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*

15037



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*

This journal is © the Owner Societies 2025

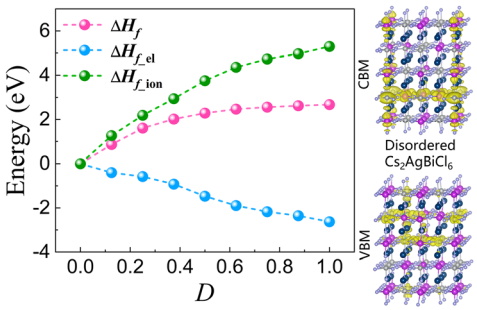
Open Access Article. Published on 17 July 2025. Downloaded on 12/12/2025 6:01:18 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

15049

Elucidating the role of lone-pair ns^2 electrons on B-site cation disordering in double halide perovskites $Cs_2AgBiCl_6$ and $Cs_2AgInCl_6$

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



15055

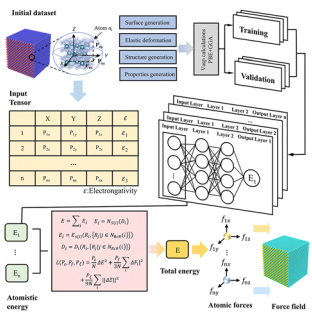
Modeling the Monty Hall decision problem with reaction kinetics

Oliver Steinbock* and Wen Zhu*

15062

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

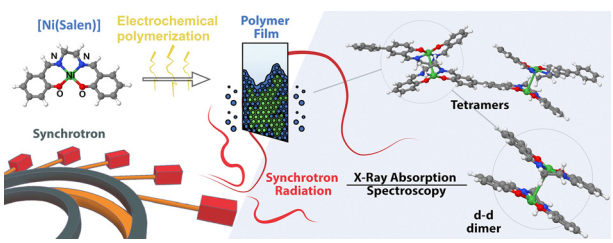
Zixuan Chen, Jixiang Ding, Shayu Song, Rongtao Shen, Jianguo Zhang,* Junfeng Xiao and Jianfeng Xu



15080

The structure of the NiO_2N_2 coordination center in the [Ni(Salen)] complex and its polymer: a comparative study by X-ray absorption spectroscopy and quantum-chemical calculations

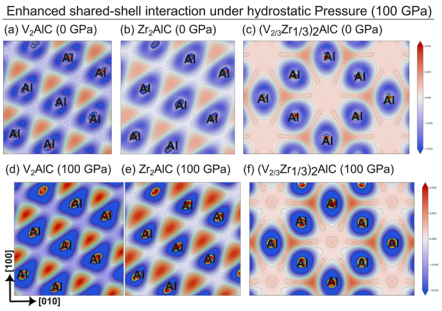
Petr M. Korusenko,* Olga V. Petrova, Anatoliy A. Vereshchagin, Oleg V. Levin, Evgeny V. Khramov, Ratibor G. Chumakov, Mikhail A. Soldatov, Konstantin P. Katin, Alexander S. Konev and Alexander S. Vinogradov



Open Access Article. Published on 17 July 2025. Downloaded on 12/12/2025 6:01:18 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

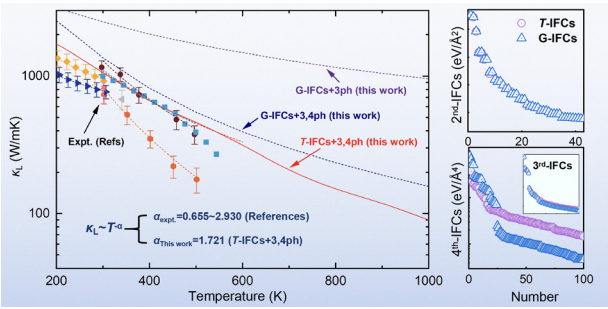
15099



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*

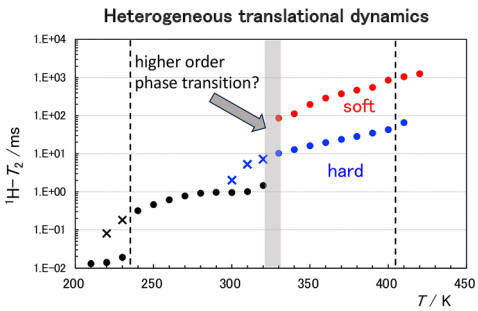
15119



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*

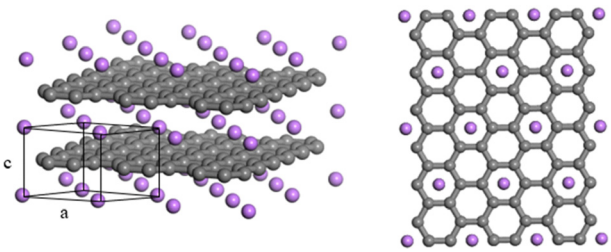
15126



Nuclear magnetic resonance study of the relationship between phase behaviour and reorientational and transrational 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

This journal is © the Owner Societies 2025

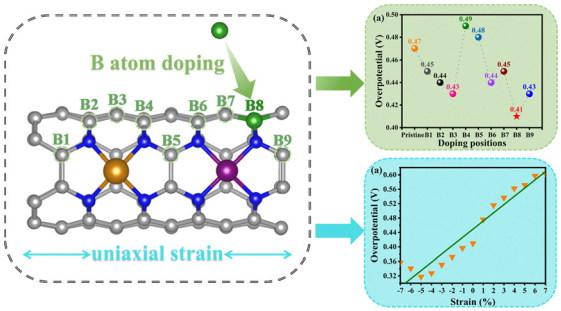
Open Access Article. Published on 17 July 2025. Downloaded on 12/12/2025 6:01:18 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

15148

Improving the activity of the oxygen evolution reaction on TiN_4–CoN_4 embedded carbon nanotubes *via* boron atom doping and applying uniaxial strain

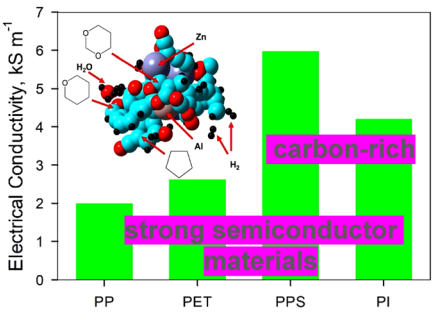
Xing-Chen Ding, Bao-Tong Cong, Wen-Hui Zhao, Zi-Qiang Deng, Long-Hui Li, Shi-Yao Liu, Zhen-Kun Tang* and Hui Zhang*



15154

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

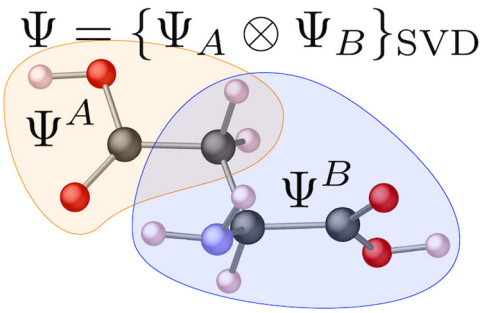
Vitaly V. Chaban* and Nadezhda A. Andreeva



15163

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

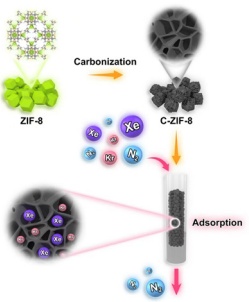
C. Sousa, X. Dong, R. Broer, T. P. Straatsma and C. de Graaf*



15176

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

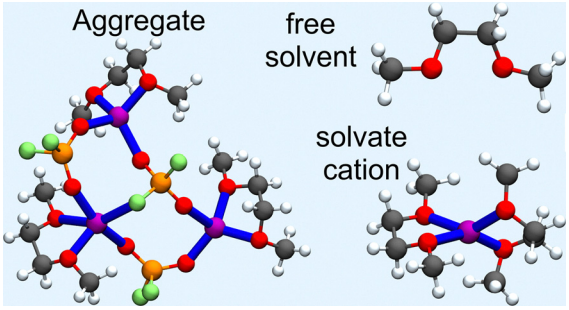
Peng Lin, Genggeng Dai, Xiaohua Liu, Yingzhe Du, Zhiguo Li, Duo Zhang, Wentao Zhou* and Fangbo Zhao*



Open Access Article. Published on 17 July 2025. Downloaded on 12/12/2025 6:01:18 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

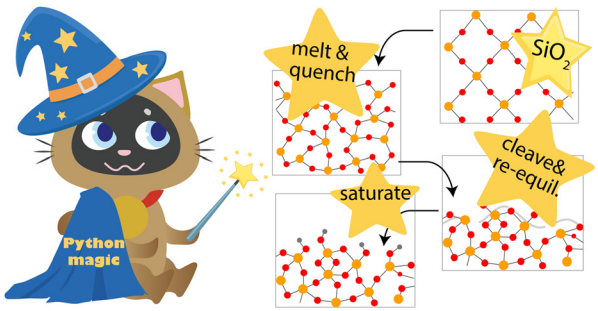
15185



Discrepant lithium transference numbers due to heterogeneous speciation

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

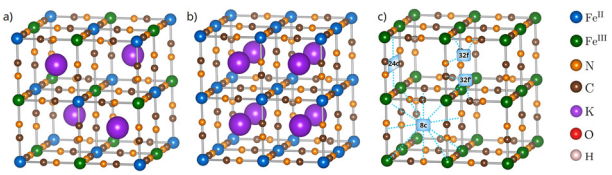
15196



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

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

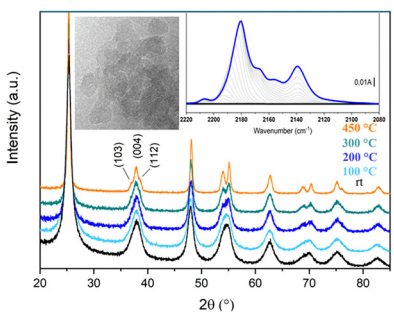
15204



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*

15213



Effect of thermal treatments on high surface area anatase TiO_2

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

This journal is © the Owner Societies 2025

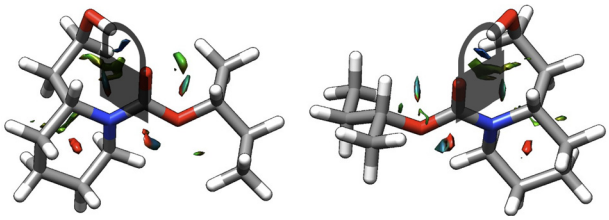
Open Access Article. Published on 17 July 2025. Downloaded on 12/12/2025 6:01:18 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

15222

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

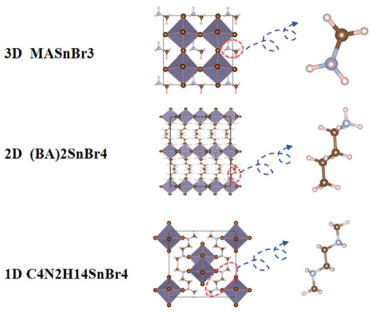
Otger Crehuet, Andrea Vázquez, Francisco J. Basterretxea, Pablo Pinacho* and Emilio J. Cocinero*



15228

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

15236

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

15237

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