

## IN THIS ISSUE

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### Cover

See Yoshiaki Kawagoe *et al.*, pp. 24250–24260. Image reproduced by permission of Yoshiaki Kawagoe from *Phys. Chem. Chem. Phys.*, 2024, 26, 24250.



### Inside cover

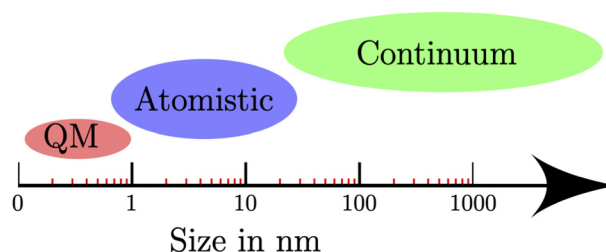
See Larissa dos Santos Silva Araújo and Leonardo Chiappisi, pp. 24246–24249. Image reproduced by permission of Institut Laue-Langevin from *Phys. Chem. Chem. Phys.*, 2024, 26, 24246. Elephants by Patryk Kosmider via Adobe Stock.

## REVIEW

24209

### Development of discrete interaction models for ultra-fine nanoparticle plasmonics

Lasse K. Sørensen,\* Valeriy S. Gerasimov, Sergey V. Karpov and Hans Ågren\*

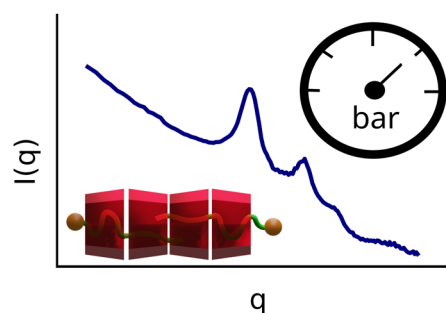


## COMMUNICATION

24246

### Effect of hydrostatic pressure on the supramolecular assembly of surfactant-cyclodextrin inclusion complexes

Larissa dos Santos Silva Araújo and Leonardo Chiappisi\*



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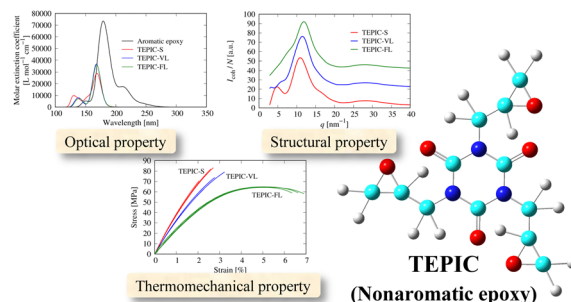


## RESEARCH PAPERS

24250

### Effects of the chain length of nonaromatic epoxy resins on thermomechanical and optical properties: experiments, and *ab initio* and molecular dynamics simulations

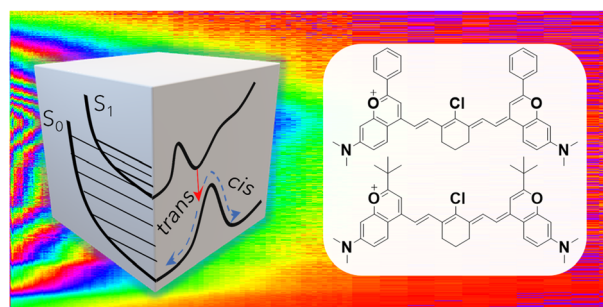
Yoshiaki Kawagoe,\* Yuuki Kinugawa, Keigo Matsumoto, Masashi Ohno, Naoki Kishimoto, Takahiko Kawai and Tomonaga Okabe



24261

### Shortwave infrared polymethine dyes for bioimaging: ultrafast relaxation dynamics and excited-state decay pathways

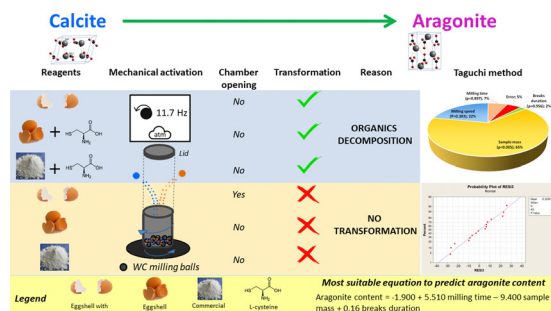
Laura M. Obloy, Steffen Jockusch and Alexander N. Tarnovsky\*



24279

### Calcite–aragonite transformation in an eggshell: a crucial role of organics and assessment of the impact of milling conditions on its extent using Taguchi design

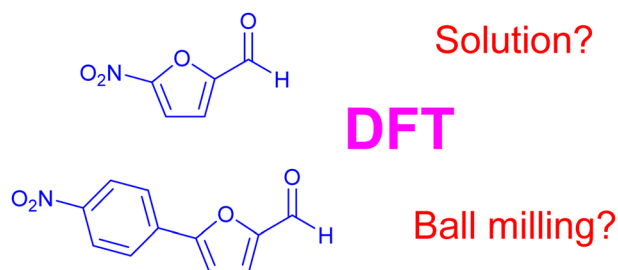
Kairat Kenges, Stephanos Karafiludis, Róbert Džunda, Imelda Octa Tampubolon, Bagdat Satybaldiyev, Franziska Emmerling and Matej Baláž\*



24288

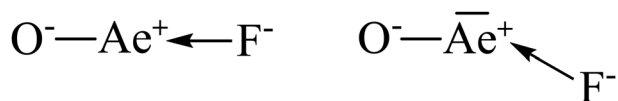
### Computational study on the mechanism for the synthesis of active pharmaceutical ingredients nitrofurantoin and dantrolene in both solution and mechanochemical conditions

Dayana M. Galeas, Iogann Tolbatov, Evelina Colacino and Felio Maseras\*



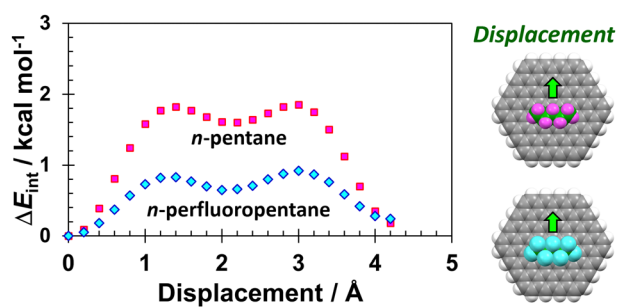
24294

### The strongest dative bond in main-group compounds. Theoretical study of $\text{O}^-\text{Ae}^+\text{F}^-$ ( $\text{Ae} = \text{Be}-\text{Ba}$ )



Lei Qin, Ruiqin Liu, Filip Sagan, Zhaoyin Zhang, Lili Zhao,\*  
Mariusz Mitoraj\* and Gernot Frenking\*

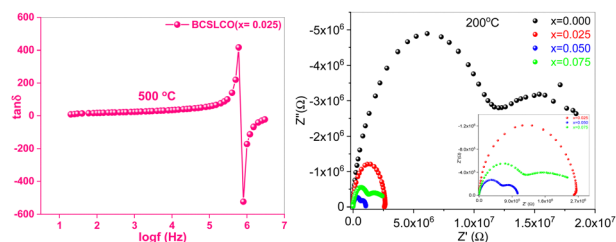
24314



### Stability of *n*-alkanes and *n*-perfluoroalkanes against horizontal displacement on a graphite surface

Yoshihiro Kikkawa\* and Seiji Tsuzuki\*

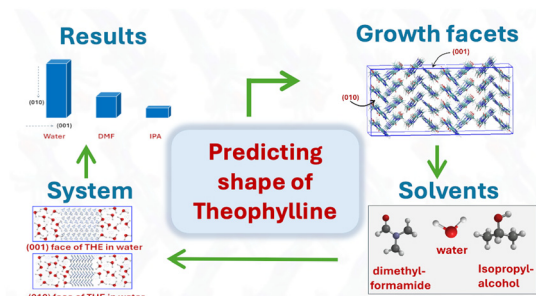
24322



### Temperature-dependent dielectric relaxations and transport properties of $\text{Sm}^{3+}$ & $\text{La}^{3+}$ doped Bi-oxide nanoparticles

Yasir Abbas, Haris Farooq Kiani, M. Kamran and  
M. Anis-ur-Rehman

24335



### Study of the solvent-dependent crystal shape of theophylline using constant chemical potential molecular dynamics simulations

Neha and Tarak Karmakar\*

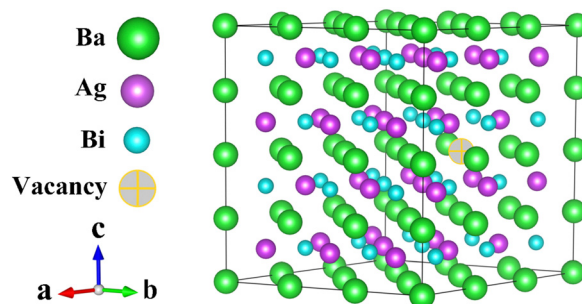


## RESEARCH PAPERS

24342

### Impact of vacancy defects on the thermal conductivity of BaAgBi: a comprehensive study using molecular dynamics simulations with neural network potentials

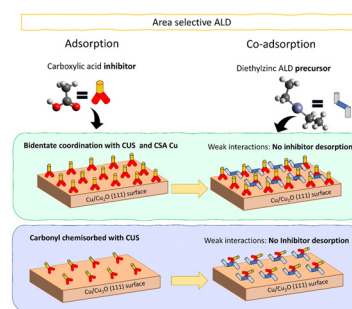
Yunzhen Du, Yuan Yao, Kunling Peng, Jizheng Duan, Changwei Hao, Yuan Tian, Wenshan Duan, Lei Yang, Ping Lin\* and Sheng Zhang\*



24352

### Understanding the role of carboxylic acid surfactants in the growth inhibition effect during area-selective atomic layer deposition: the case of ZnO growth on Cu and Cu<sub>2</sub>O

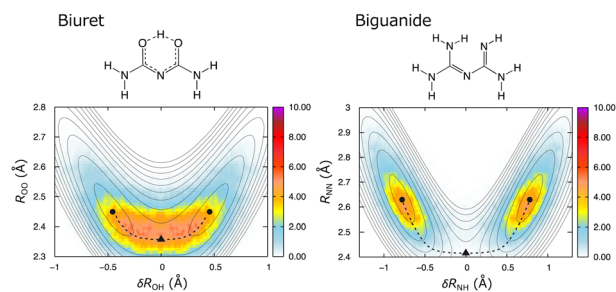
L. E. López-González\*, R. Ponce-Pérez, H. Tiznado\* and J. Guerrero-Sánchez\*



24364

### Nuclear quantum effects on the intramolecular hydrogen bonds in biuret and biguanide

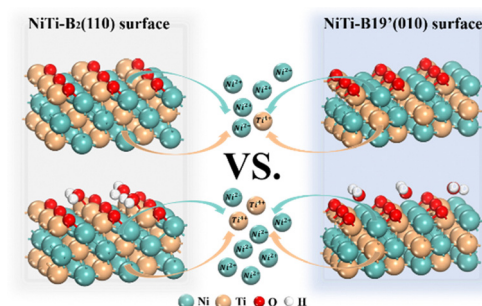
Kotomi Nishikawa, Hikaru Tanaka, Kazuaki Kuwahata, Masanori Tachikawa and Taro Udagawa\*



24370

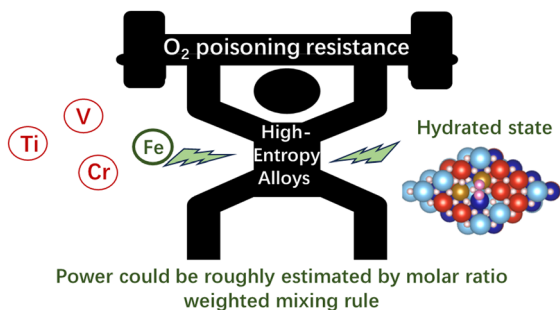
### Effects of adsorption of O<sub>2</sub> and H<sub>2</sub>O molecules on the corrosion behavior of the NiTi alloy surface: a DFT investigation

Xiaoting Wang, Dong Xie\*, MingXi Hou, Min Guan and Yongxiang Leng\*



## RESEARCH PAPERS

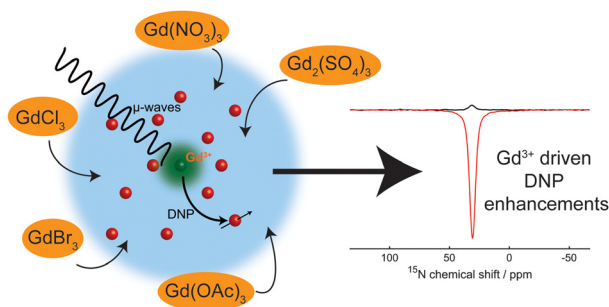
24384



### Theoretical study on the surface poisoning of high-entropy alloys during hydrogen storage cycles: the effect of metal elements and phases

Ming Jiang, Yixin Yang, Hongjiao Li\* and Bin Liang

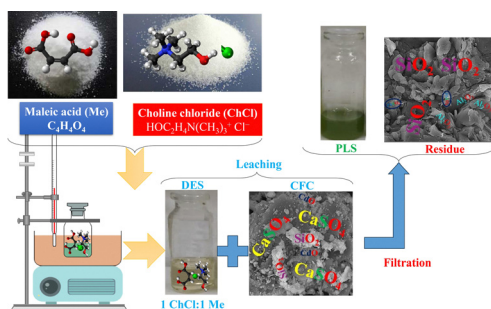
24395



### Optimisation of dynamic nuclear polarisation using "off-the-shelf" Gd(III)-based polarising agents

Daniel J. Cheney, Paolo Cerreia Vioglio, Adam Brookfield and Frédéric Blanc\*

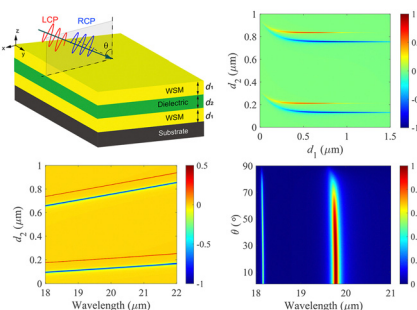
24407



### Green leaching of cold filter cakes using choline chloride–maleic acid deep eutectic solvent and molecular dynamics simulation

Bahram Behnajady,\* Matin Najafi and Saeid Karimi\*

24423



### Weyl semimetal/dielectric/Weyl semimetal stack for highly circularly polarized thermal radiation

Xin Cui, Qi Fang, Liming Qian and Gaige Zheng\*

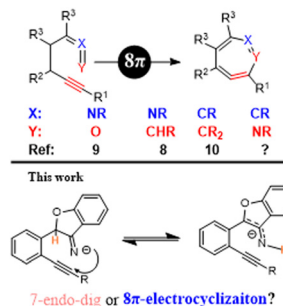


## RESEARCH PAPERS

24431

**Anionic aza  $8\pi$ -electrocyclization as an unprecedented pathway *versus* 7-endo-dig: DFT study on the mechanism of base-catalyzed benzofuroazepine synthesis *via* cyclization of (2-alkynylbenzyl)oxy nitriles**

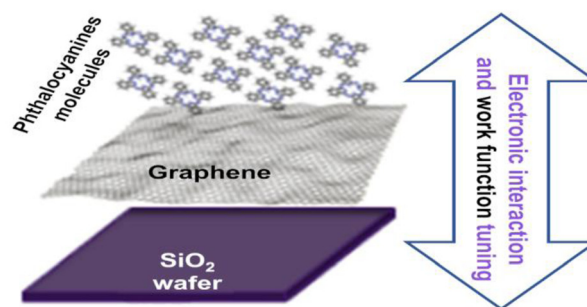
Omid Amiri and Ayoob Bazgir\*



24438

**Investigation into electronic interaction and work function tuning of phthalocyanine molecules and graphene interfaces**

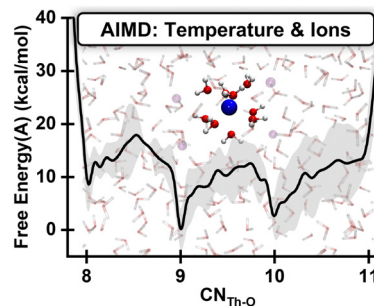
Yunier Garcia-Basabe,\* Matheus Suenson Cardoso, Bruno da Silva Lima, Cesar D. Mendoza, Fernando Lázaro Freire Junior and Dunieskys G. Larrude\*



24447

**Structures of Th<sup>4+</sup> aqueous solutions: insights from AIMD and metadynamics simulations**

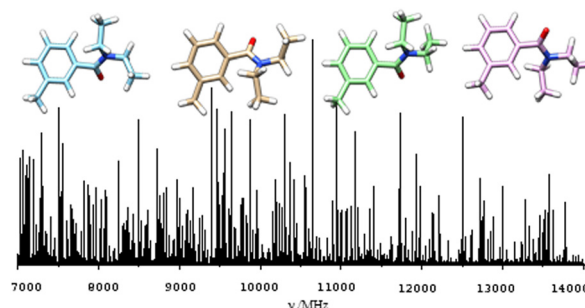
Yang He, Jun-Bo Lu, Yang-Yang Zhang, Han-Shi Hu\* and Jun Li\*



24455

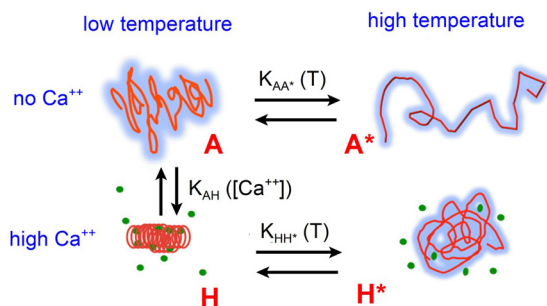
**Shape and interactions of the synthetic repellent DEET**

Otger Crehuet, Andrea Vázquez, Pablo Pinacho, Aran Insausti, Elena R. Alonso, Francisco J. Basterretxea and Emilio J. Cocinero\*



## RESEARCH PAPERS

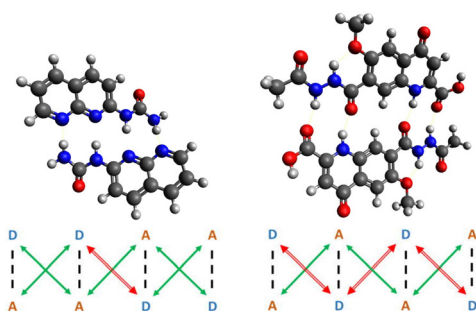
24461



The effect of Ficoll 70 on thermally-induced and chemically-induced conformational transitions of an RTX protein is quantitatively accounted for by a unified excluded volume model

Alexandre Chenat\* and Allen P. Minton\*

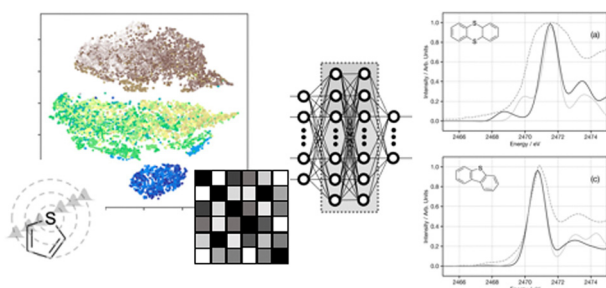
24470



Attractive acceptor-acceptor interactions in self-complementary quadruple hydrogen bonds for molecular self-assembly

Usman Ahmed, Christopher D. Daub, Dage Sundholm\* and Mikael P. Johansson\*

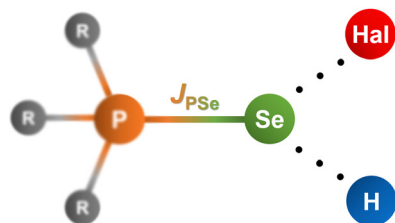
24477



Partial density of states representation for accurate deep neural network predictions of X-ray spectra

Clelia Middleton, Basile F. E. Curchod and Thomas J. Penfold\*

24488



Phosphine selenides are universal NMR probes for HBs and XBs

Phosphine selenides: versatile NMR probes for analyzing hydrogen OH...Se and halogen I...Se bonds

Anton S. Zakharov, Danil V. Krutin, Pavel O. Mosalyov, Elena Yu. Tupikina, Alexander S. Antonov, Peter M. Tolstoy and Valeriya V. Mulloyarova\*

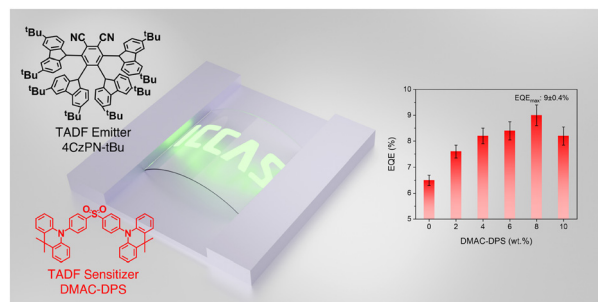


## RESEARCH PAPERS

24498

Achieving 9% EQE in light-emitting electrochemical cells *via* a TADF-sensitized fluorescence strategy

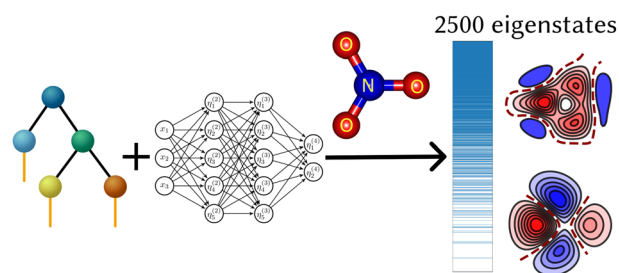
Zeyang Zhou, Qingda Chang, Rui Chen, Pengfei Jin, Baipeng Yin,\* Chuang Zhang\* and Jiannian Yao



24506

2500 vibronic eigenstates of the NO<sub>3</sub> radical

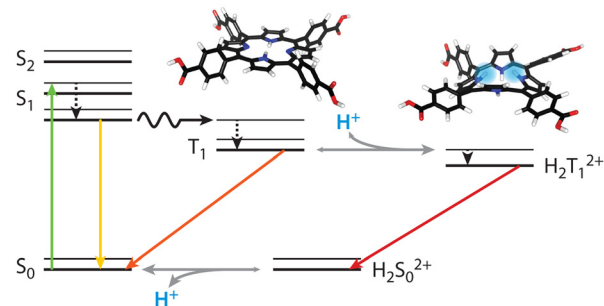
Henrik R. Larsson\* and Alexandra Viel



24524

## Porphyrins on acid: kinetics of the photoinduced-protonation of tetrakis(4-carboxyphenyl)-porphyrin

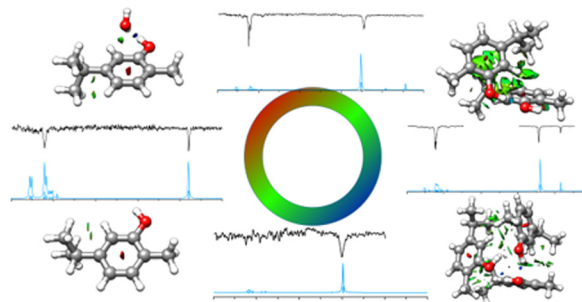
P. Tim Prins, Dorota Rutkowska-Zbik, Sonja Pullen and Bettina Baumgartner\*



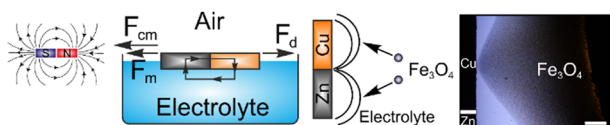
24533

## Exploration of carvacrol aggregation by laser spectroscopy

Paúl Pinillos, Fernando Torres-Hernández, Imanol Usabiaga, Pablo Pinacho\* and José A. Fernández\*



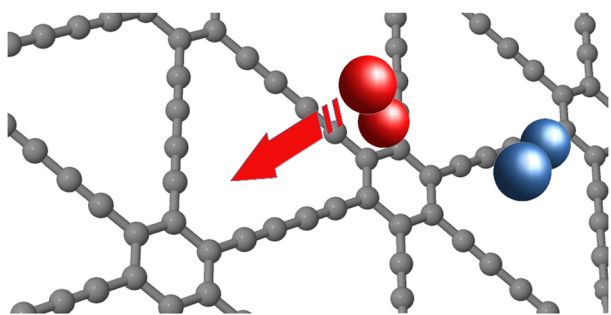
24542



### Chemical magnetism – surface force to move motors

Boris Kichatov,\* Alexey Korshunov and Vladimir Sudakov

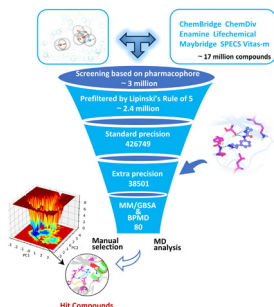
24553



### Separation of oxygen from nitrogen using a graphdiyne membrane: a quantum-mechanical study

Maryam A. Rafiei,\* José Campos-Martínez, Massimiliano Bartolomei, Fernando Pirani, Ali Maghari and Marta I. Hernández\*

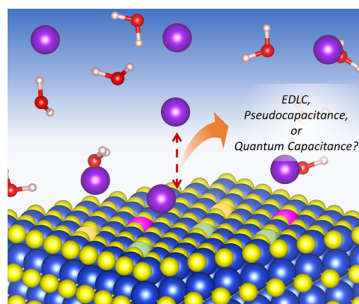
24564



### Discovery of a urea-based hit compound as a novel inhibitor of transforming growth factor- $\beta$ type 1 receptor: *in silico* and *in vitro* studies

Yaxin Li, Sisi Liu, Zhuoya Wang, Xiaoli Wang, Jiamin Xu, Keke Yao, Ranran Zhang, Chenxuan Lu, Zhigang Wu and Liming Hu\*

24577



### Unveiling the role of dopants in boosting CuS supercapacitor performance: insights from first-principles calculations

Muhammad Alief Irham, Fakhrian Hanif Tejo Baskoro, Ahmad Al Ghiffari, Darul Roni Rodiansyah, Arie Wibowo, Fahdzi Muttaqien and Ferry Iskandar\*

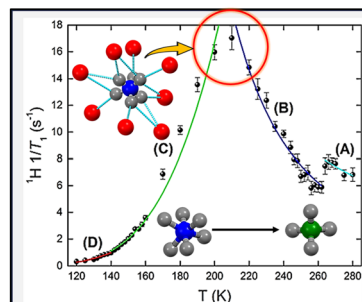


## RESEARCH PAPERS

24585

### Understanding the motional dynamics of the ammonium ion in the mechanism of multiferroicity of Cr(v) peroxochromates: a $^1\text{H}$ NMR study

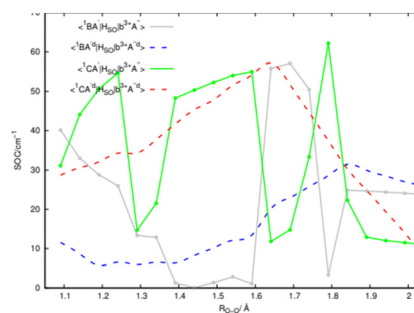
Raghabendra Samantaray,\* Debashis Acharya, Anulipsa Priyadarshini, Rojalini Sahu,\* T. Besara and Naresh S. Dalal



24591

### Fully quantal description of combined internal conversion and intersystem crossing processes in the smallest Criegee intermediate $\text{CH}_2\text{OO}$

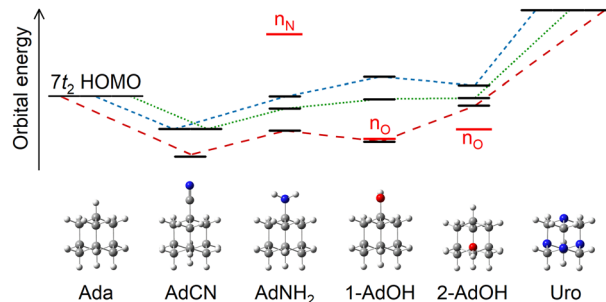
Behnam Nikoobakht\* and Horst Köppel



24607

### Photoelectron spectra of functionalized adamantanes

Parker Crandall, Simone Stahl, Andrea Merli, Marko Förstel and Otto Dopfer\*



24624

### Can the Kohn–Sham gap be larger than the fundamental gap?

Kossi Kety\* and Daniel Joubert

#### Can the Derivative Discontinuity be negative in Kohn–Sham DFT ?

DFT on the Hubbard dimer + self-consistent scheme to compute the KS potential.

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_k v_k n_k$$

Repulsion constant  $U$ , hopping parameter  $t$  and onsite potential  $v_k$

Derivation of the Janak's theorem on a lattice:  $\frac{\partial E}{\partial p_i} = \epsilon_i \Rightarrow I = -\epsilon^{\text{homo}}$ ;  $E$  the total energy  $I$  is the ionization energy,  $A$  the electron affinity.

for  $U = 5$ ,  $t = 1/2$ ,  $\Delta_{xc}$  can be negative. This behaviour remains to be seen in a real system with Coulombic interactions.

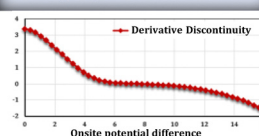
The Kohn–Sham gap:

$$E_g^{KS} = \epsilon^{\text{lumo}} - \epsilon^{\text{homo}}$$

The Fundamental gap:  $E_g = I - A$

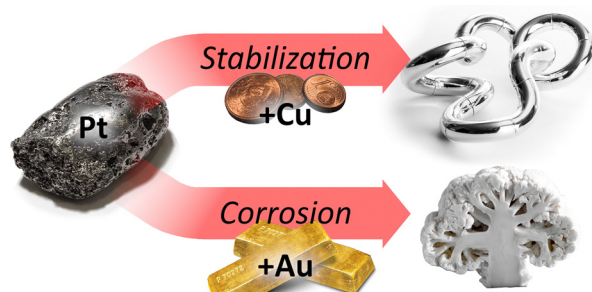
The derivative discontinuity:

$$\Delta_{xc} = E_g - E_g^{KS} = -A - \epsilon^{\text{lumo}}$$



## RESEARCH PAPERS

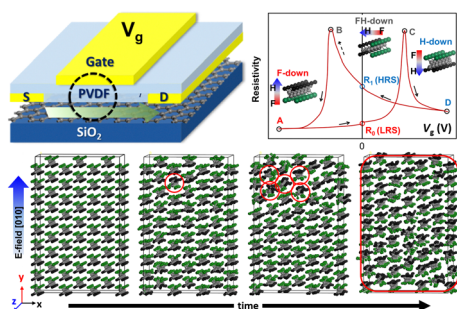
24631



### Why alloying with noble metals does not decrease the oxidation of platinum: a DFT-based *ab initio* thermo-dynamics study

Alexander Kafka and Franziska Hess\*

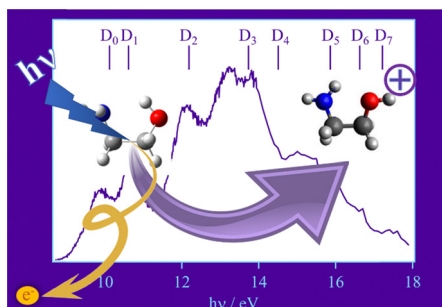
24649



### Resistance switching of graphene by gate-controlled polarization reorientation of polyvinylidene fluoride in a field effect transistor

Jinhee Lee, Nodo Lee, Yves Lansac and Yun Hee Jang\*

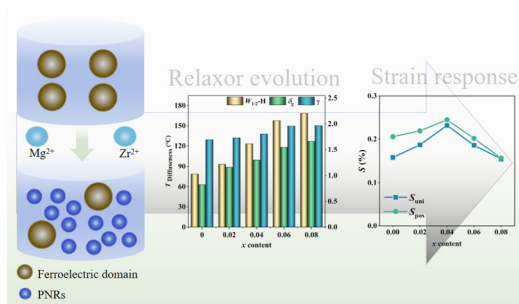
24656



### Photoelectron spectrum and breakdown diagram of ethanolamine: conformers, excited states, and thermochemistry

S. Kechoindi, S. Ben Yaghlane, M. Mogren Al Mogren, A. Bodi\* and M. Hochlaf\*

24667



### Strain evolution from the ferroelectric to the relaxor state in $(0.67 - x)\text{BiFeO}_3 - 0.33\text{BaTiO}_3 - x\text{Bi}(\text{Mg}_{0.5}\text{Zr}_{0.5})\text{O}_3$ lead-free ceramics

Jiaqing Feng, Yiting Zhang, Xilong Song, Zixin Liu, Chen Liao, Lin Zhao, Bo Wu,\* Hong Tao and Jian Ma

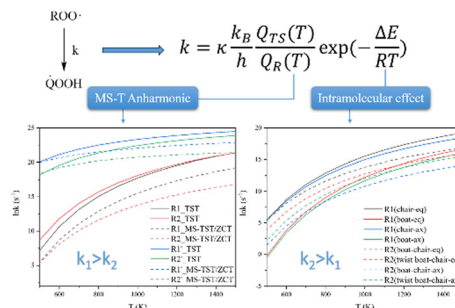


## RESEARCH PAPERS

24676

### Theoretical kinetic studies on intramolecular H-migration reactions of peroxy radicals of diethoxymethane

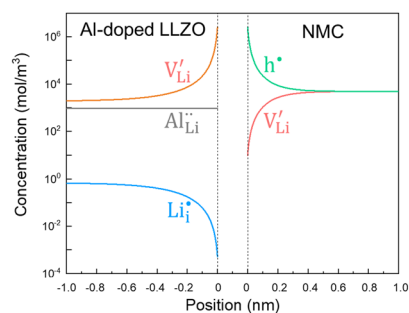
Siyu Chen, Juanqin Li, Quan Zhu\* and Zerong Li



24689

### Space charge effects in mixed ionic–electronic conducting electrodes for solid-state batteries

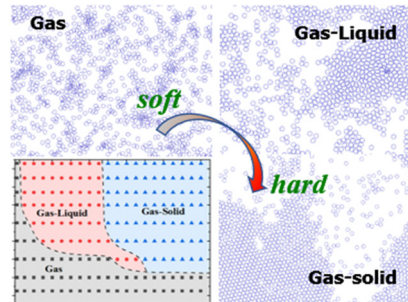
Shu-Han Chen and Chia-Chin Chen\*



24699

### Deformation-induced phase separation of active vesicles

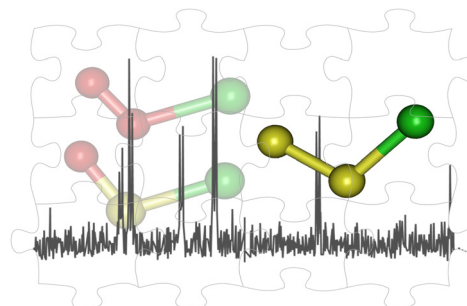
Yi-yang Jin, Yan Jin, Zi-xuan Shi, Wen-de Tian,\* Tian-hui Zhang\* and Kang Chen\*



24709

### Fourier-transform microwave spectroscopy of the CISS radical

Ching-Hua Chang, Chen-Han Tsai and Yasuki Endo\*



## CORRECTIONS

24714

**Correction: The Lennard-Jones potential: when (not) to use it**

Xipeng Wang, Simón Ramírez-Hinestrosa, Jure Dobnikar and Daan Frenkel\*

24716

**Correction: Water adsorption lifts the (2 × 1) reconstruction of calcite(104)**

Jonas Heggemann, Simon Aeschlimann, Tobias Dickbreder, Yashasvi S. Ranawat, Ralf Bechstein, Angelika Kühnle, Adam S. Foster\* and Philipp Rahe\*

