

## IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 27(38) 20381–20954 (2025)



### Cover

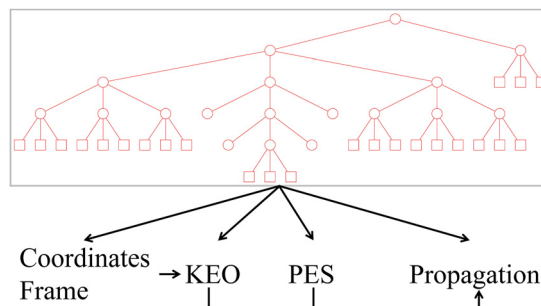
See Taro Udagawa *et al.*, pp. 20474–20483. Image reproduced by permission of Taro Udagawa from *Phys. Chem. Chem. Phys.*, 2025, 27, 20474.

## PERSPECTIVE

20397

### A hierarchical wavepacket propagation framework via ML-MCTDH for molecular reaction dynamics

Xingyu Zhang and Qingyong Meng\*

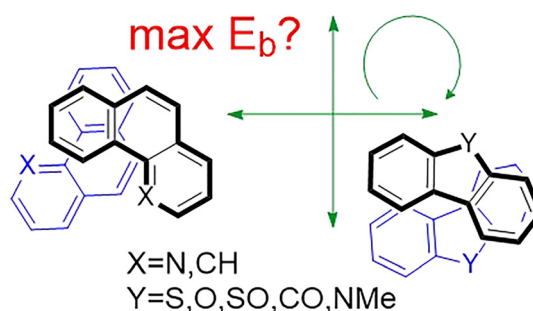


## TUTORIAL REVIEW

20421

### An efficient workflow for generation of conformational ensembles of density functional theory quality: dimers of polycyclic (hetero-)aromatics

Jessica J. Ortlieb, Nathanael J. King and Alex Brown\*



# Industrial Chemistry & Materials

GOLD OPEN ACCESS

Focus on industrial chemistry  
Advance material innovations  
Highlight interdisciplinary feature

Published on 02 October 2015. Downloaded from rsc.li/indchemmater



Innovative.  
Interdisciplinary.  
Problem solving

APCs currently waived

Learn more about ICM  
Submit your high-quality article

 @IndChemMater

 @IndChemMater

[rsc.li/icm](http://rsc.li/icm)

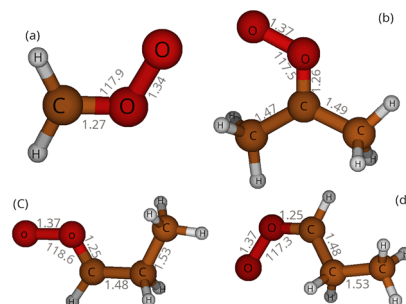


## REVIEW

20433

## UV photodissociation and population dynamics of some important Criegee intermediates

Behnam Nikoobakht, Maximilian F. S. J. Menger and Horst Köppel\*

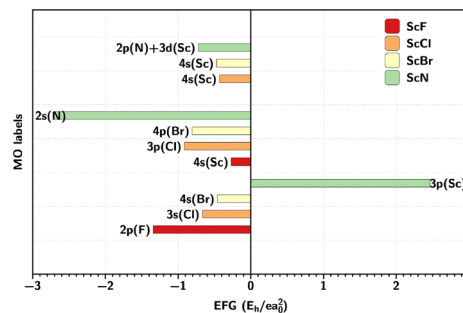


## COMMUNICATIONS

20453

Nuclear electric quadrupole moment of  $^{45}\text{Sc}$ : reconfirmation and extension to diatomic ScN

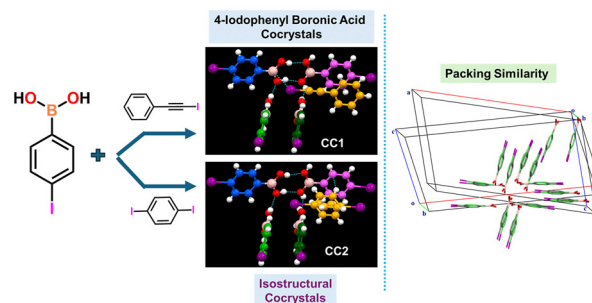
Jean-Pierre Dognon\* and Pekka Pyykkö\*



20456

## Quantitative insights into the role of halogen and triel bonds in the formation of isostructural co-crystals of 4-iodophenyl boronic acid

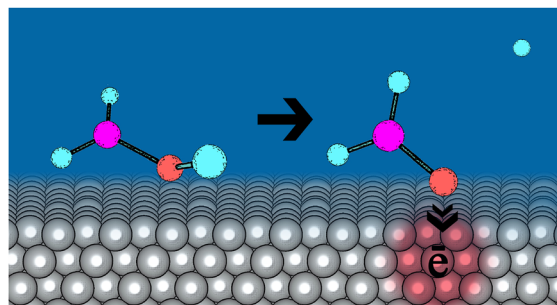
Koushik Mandal, Ajay Suresh and Deepak Chopra\*



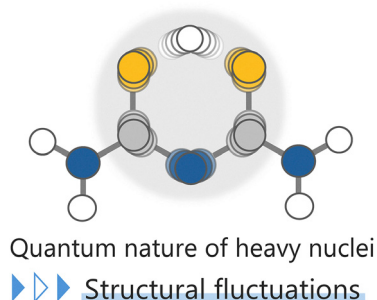
20468

## Computational investigation of charge transfer from hydroxymethyl radicals to metal surfaces suspended in water

Basil Raju Karimadom, Dan Meyerstein, Amir Mizrahi and Haya Kornweitz\*



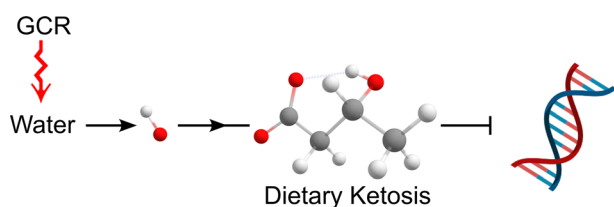
20474



### Nuclear quantum effects on intramolecular hydrogen bonds and backbone structures in biuret analogues

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

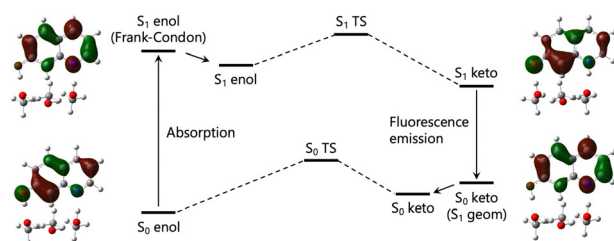
20484



### Feasibility of the reaction between (*R*)-3-hydroxybutyrate & hydroxyl radicals

Peter A. C. McPherson,\* Ruaidhrí MacDonnell and Ben M. Johnston

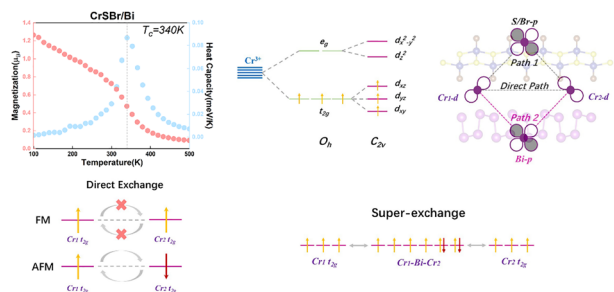
20493



### A multi-component density functional study on quantum effects of hydrogen nuclei on ground-state and excited-state proton transfer reactions in 7-hydroxyquinoline

Taro Udagawa,\* Hinata Nagasaka, Yusuke Kanematsu,\* Takayoshi Ishimoto and Masanori Tachikawa

20500



### Enhanced Curie temperature of ferromagnetic CrSBr by interfacial coupling with elemental two-dimensional ferroelectrics: triggering a new p–d super-exchange coupling path

Xiaotong Zhou and Baozeng Zhou\*

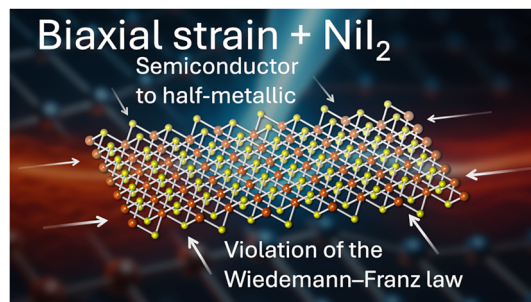


## RESEARCH PAPERS

20509

**Strain-induced half-metallicity and giant Wiedemann–Franz violation in monolayer  $\text{NiI}_2$** 

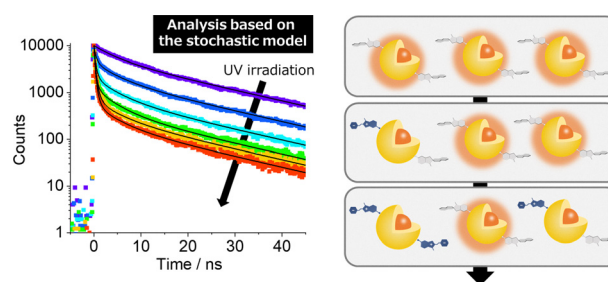
Jhon W. González\* and Luis Rosales



20519

**Stochastic model analysis of luminescence switching in hybrid systems of CdSe/CdS quantum dots–spiropyran molecular photoswitches**

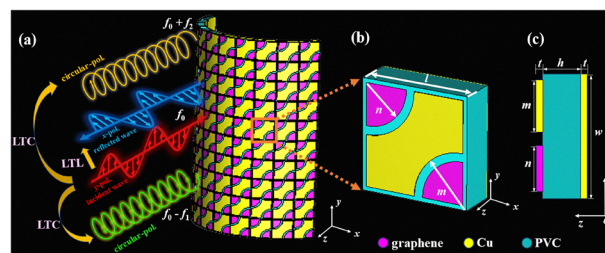
Sho Shishido, Moe Yamamoto, Daichi Eguchi\* and Naoto Tamai\*



20527

**A flexible linear circular bipolarization conversion metasurface based on graphene**

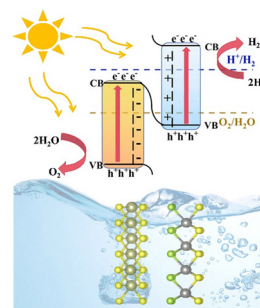
Changfeng Fu, Yu Zhu, Bo Yang, Mingzhu Ma, Mengge Lv, Shaohua Dong and Lianfu Han\*



20537

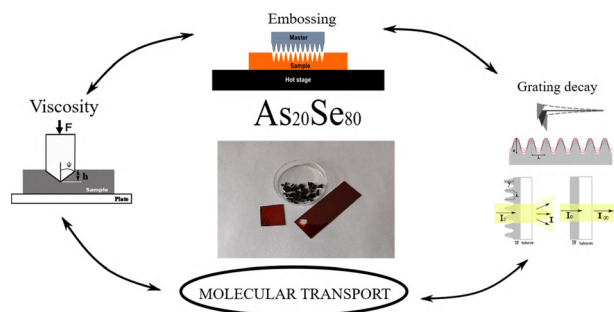
**Design of Z-scheme WSe– $\text{XS}_2$  ( $X = \text{Zr}$  and  $\text{Hf}$ ) heterostructures as photocatalysts for efficient solar water splitting**

Wei Zhang, Zheng Dai, Lina Bai\* and Yuan Zhao



## RESEARCH PAPERS

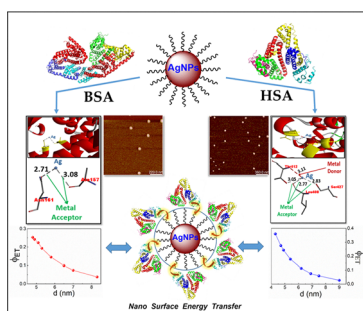
20546



### Surface kinetics and viscosity in amorphous $\text{As}_{20}\text{Se}_{80}$ : a comparative study of bulk and thin films prepared by thermal evaporation and spin-coating

Michaela Včeláková,\* David Vaculik, Michal Kurka, Jiri Jancalek, Stanislav Slang, Torsten Wieduwilt, Markus A. Schmidt, Hiroyo Segawa and Jaroslav Barták

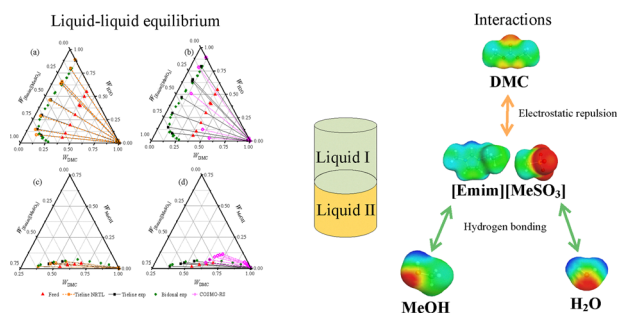
20557



### Photophysical, thermodynamic and molecular docking studies on the comparative binding interaction of biosynthesized silver nanoparticles with homologous serum proteins: a comprehensive analysis of the interaction mechanisms at both the molecular and nanoscale levels

Amar Ghosh, Himal Das, Murugesan Panneerselvam, Manorama Ghosal, Rapti Goswami, Luciano T. Costa, Dulal Senapati, Ujjal Kumar Sur\* and Suman Das\*

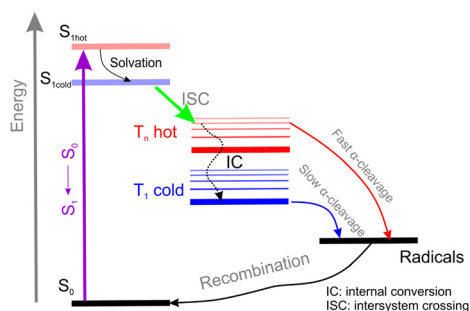
20577



### Liquid-liquid equilibrium and modelling insight: molecular interaction analysis of water + methanol + dimethyl carbonate + 1-ethyl-3-methylimidazolium methanesulfonate ternary systems

Juho-Pekka Laakso,\* Behnaz Asadzadeh, Petri Uusi-Kyyny and Ville Alopaeus

20592



### Uncovering the photoexcited dynamics in bis(acyl)phosphine oxide photoinitiators

Marius Navickas,\* Edvinas Skliutas, Joseph Kölbel, Ricardo J. Fernández-Terán,\* Mangirdas Malinauskas and Mikas Vengris

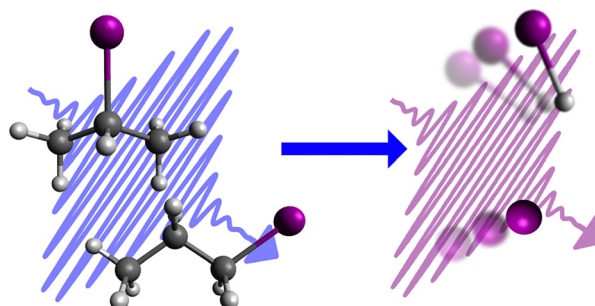


## RESEARCH PAPERS

20602

### Time-resolved momentum imaging of UV photodynamics in structural isomers of iodopropane probed by site-selective XUV ionization

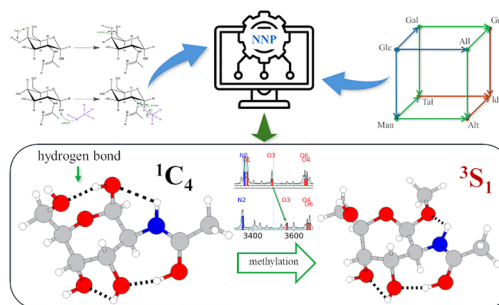
Felix Allum,\* Yoshiaki Kumagai, Kiyonobu Nagaya, James R. Harries, Hiroshi Iwayama, Mathew Britton, Philip H. Bucksbaum, Michael Burt, Mark Brouard, Briony Downes-Ward, Taran Driver, David Heathcote, Paul Hockett, Andrew J. Howard, Jason W. L. Lee, Yusong Liu, Edwin Kukk, Joseph W. McManus, Dennis Milešević, Russell S. Minns, Akinobu Niozu, Johannes Niskanen, Andrew J. Orr-Ewing, Shigeki Owada, Patrick Robertson, Daniel Rolles, Artem Rudenko, Kiyoshi Ueda, James Unwin, Claire Vallance, Tiffany Walmsley, Michael N. R. Ashfold and Ruairidh Forbes\*



20614

### Conformational analysis of protonated *N*-acetyl hexosamines: unexpected methylation effects from first-principles and machine learning

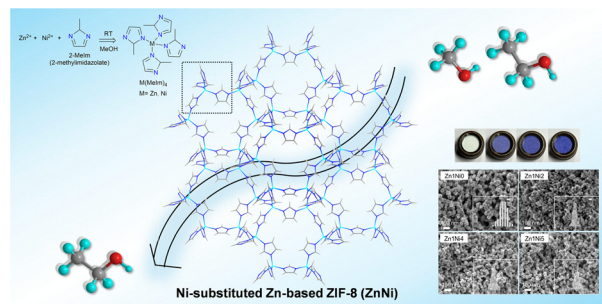
Kenee Kaiser Suyo Custodio,\* Truc Quyen Vo Thi, Huu Trong Phan, Pei Kang Tsou and Jer-Lai Kuo\*



20625

### Tailoring Zn-based zeolitic imidazolate frameworks via Ni substitution: a strategy for enhanced selective alcohol adsorption and separation

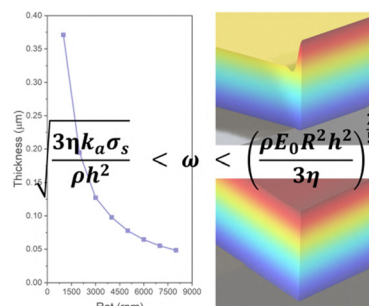
Panyapat Ponchai, Kanyaporn Adpakpang, Yollada Inchongkol, Kajjana Boonpalit, Suttipong Wannapaiboon and Sareeya Bureekaew\*



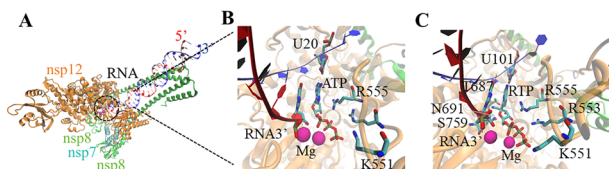
20636

### Theoretical design of critical spin speed and the process window for spin-coated self-assembled monolayers

Zeshuo Meng,\* Runlin Zhang, Zhengyan Du,\* Meiyang Wang\* and Haoteng Sun\*



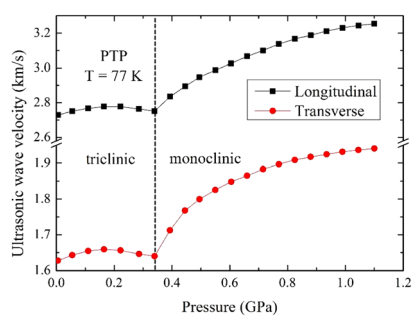
20645



### The fidelity control of nucleotide selectivity in SARS-CoV-2 RdRp through amino acid mutations *via* molecular dynamics simulations

Hong Hu, Hongqiong Liang, Jin Yu, Liqiang Dai, Zixuan Lu and Chunhong Long\*

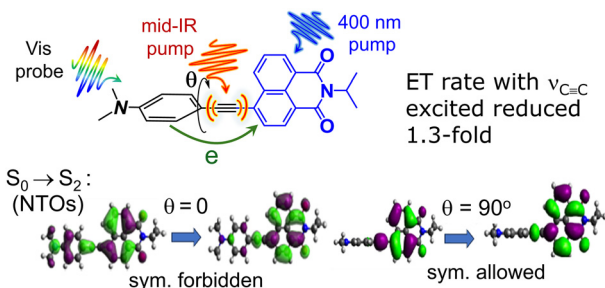
20661



### Ultrasonic study of terphenyls under high pressure: 2nd order phase transition in *para*-terphenyl and glass transition in *ortho*-terphenyl

Igor V. Danilov,\* Elena L. Gromnitskaya and Vadim V. Brazhkin

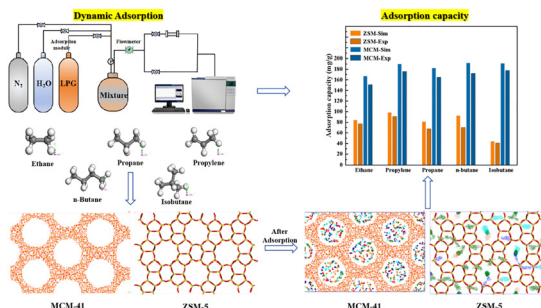
20668



### Photo-induced electron transfer dynamics and its mid-IR modulation of an ethyne bridged donor–acceptor complex

Kasun C. Mendis, Xiao Li, Jesús Valdiviezo, Susannah D. Cox, Peng Zhang, Nisansala S. S. Thalaththani Rallage, Tong Ren, David N. Beratan\* and Igor V. Rubtsov\*

20680



### Adsorption performance of ZSM-5 and MCM-41 molecular sieves for light hydrocarbons and liquefied petroleum gas

Wenxing Qi, Tongyuan Liu, Lihong Nie, Hongtao Jiang and Beifu Wang\*

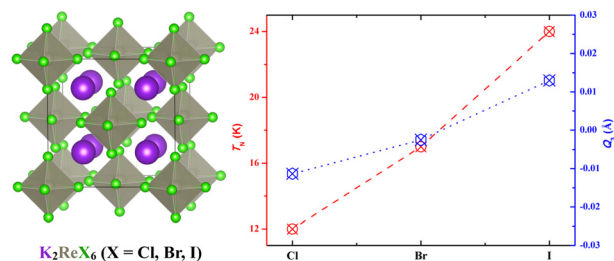


## RESEARCH PAPERS

20699

### Magnetic properties and spin–orbit coupling-driven Jahn–Teller distortions in $K_2\text{ReX}_6$ ( $X = \text{Cl}, \text{Br}$ and $\text{I}$ ) with a half-filled $5d-t_{2g}^3$ shell

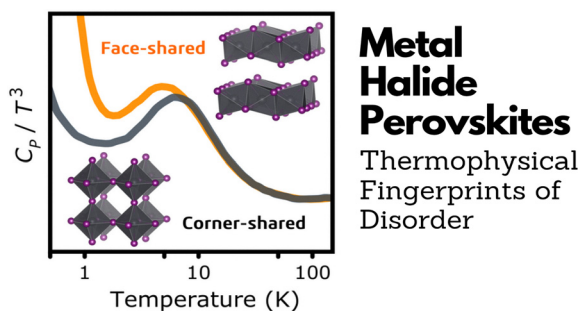
Yixuan Du, Yaoyao Hao, Xianfeng Hao,\* Yongchao Jia, Keju Sun and Yuanhui Xu\*



20709

### Low-energy modes and localized excitations in metal halide perovskites: insights from heat capacity

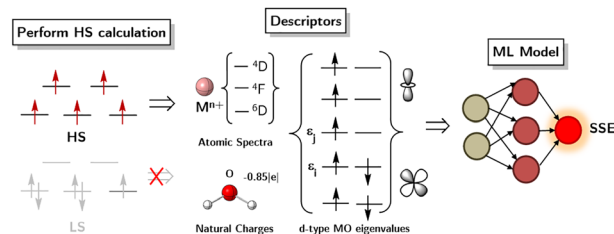
Ana Arauzo,\* Pelayo Marin-Villa, Kacper Druzbicki, María Concepción Sánchez and Felix Fernandez-Alonso\*



20717

### Leveraging high-spin DFT features for prediction of spin state gaps in 3d transition metal complexes

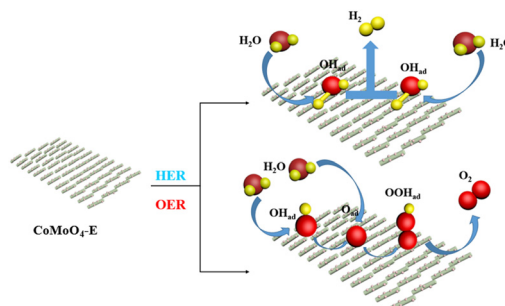
Anuj Kumar Ray, Sandeep Nagar, Girish Varma,\* U. Deva Priyakumar and Ankan Paul\*



20726

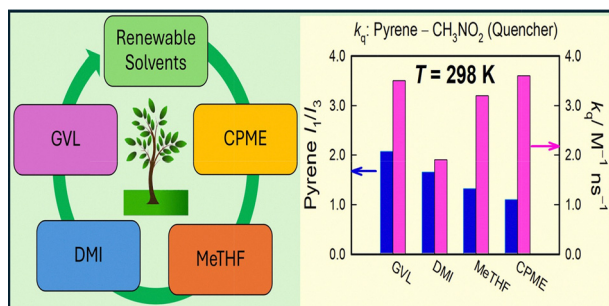
### Hydroxyl-regulated $\text{CoMoO}_4$ nanotubes as an efficient bifunctional electrocatalyst for the hydrogen/oxygen evolution reaction

Heng Ke, Yaya Xie, Yi Luo, Yinhong Gao, Lan Yin, Jun Fu, Liangzhe Chen, Wentao Tang, Youbing Zhang, Jing Ding, Zhe Fu and Faquan Yu\*



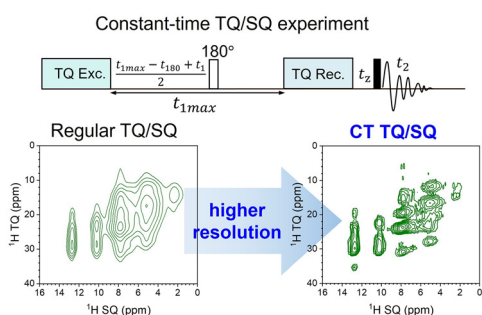
## RESEARCH PAPERS

20735

Investigation of solute solvation within renewable solvents *via* pyrene fluorescence

Anuj Sharma and Siddharth Pandey\*

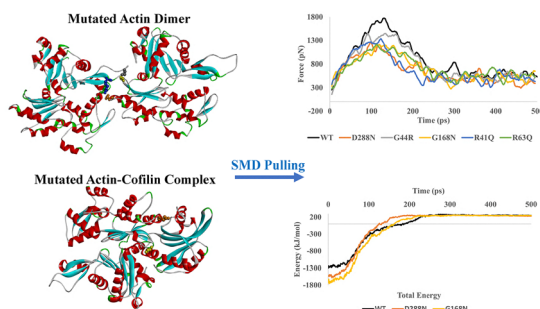
20745



## Constant-time evolution enhances the resolution of triple-quantum NMR spectroscopy at fast MAS

Yixiang Yan, Zhiwei Yan, Yusuke Nishiyama and Rongchun Zhang\*

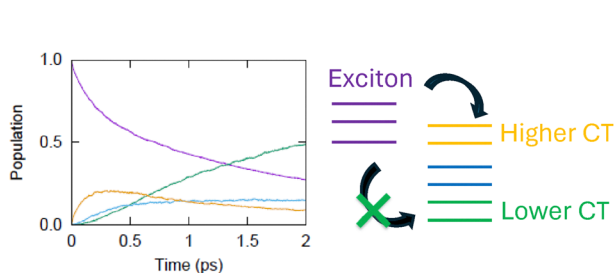
20754



## Computational insights into the effect of mutation on actin-actin dimer and actin-related binding protein interactions

Danial Sedighpour, Farzan Ghalichi and Iman Zoljanahi Oskui\*

20765



## Exciton dissociation pathways in donor/acceptor blends studied by the wave packet dynamics approach

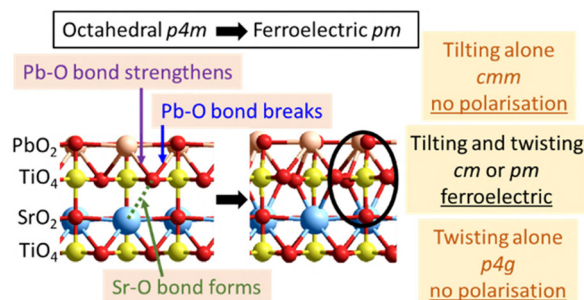
Takatoshi Fujita\* and Misa Nozaki



20773

### Chemical control of polymorphism and ferroelectricity in $\text{PbTiO}_3$ and $\text{SrTiO}_3$ monolayers and bilayers

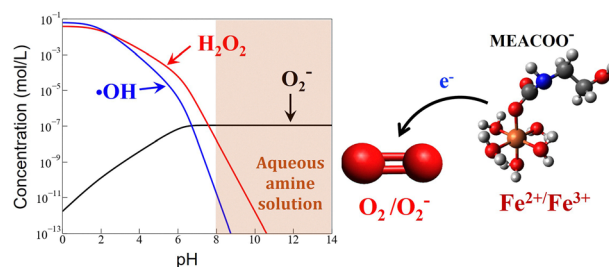
Shaowen Xu, Jeffrey R. Reimers,\* Fanhao Jia and Wei Ren\*



20787

### Revealing the dominant reactive oxygen species in aqueous amine solutions for carbon capture

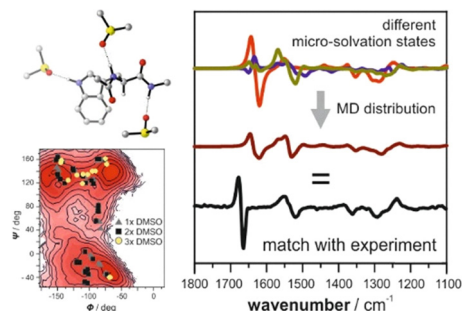
Dipam Patel, Jiwon Yu and Gyeong S. Hwang\*



20794

### A VCD study on micro-solvation and self-aggregation of *N*-acetyl tryptophan propylamide

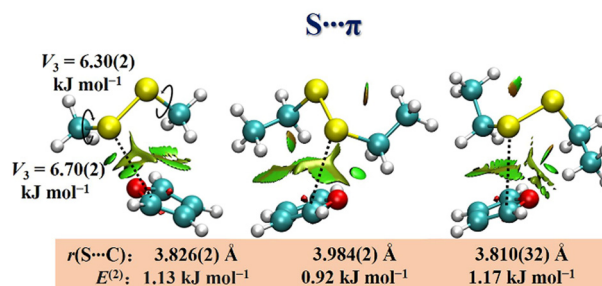
Dilber Tan, Veronika Stoianova and Christian Merten\*



20802

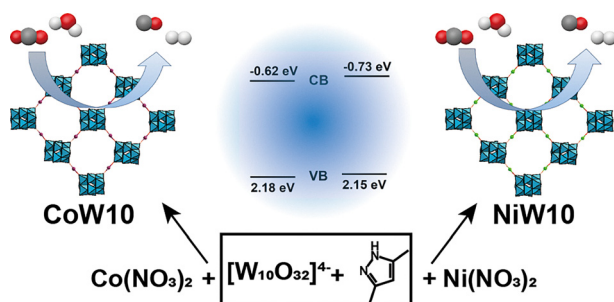
### Unraveling the $\text{S}\cdots\text{S}\cdots\pi$ interactions in furan-disulfide heterodimers: insights from microwave spectroscopy and *ab initio* computations

Fang Shen, Liuting Wang, Renhua Chen, Wenqin Li, Yuting Li, Yan Feng, Tao Lu,\* Walther Caminati, Alberto Lesarri and Gang Feng\*



## RESEARCH PAPERS

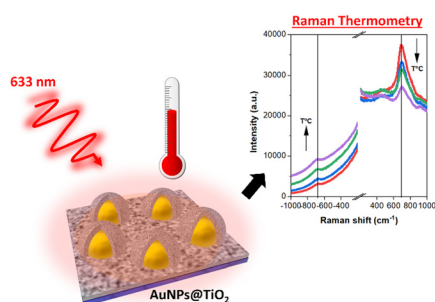
20810



### Visible-light driven photoreduction of carbon dioxide to syngas with decatungstate-based metal–organic frameworks

Hua Li, Yaomei Fu, Shuangxue Wu, Li Liu,\* Xinlong Wang, Chao Qin\* and Zhongmin Su

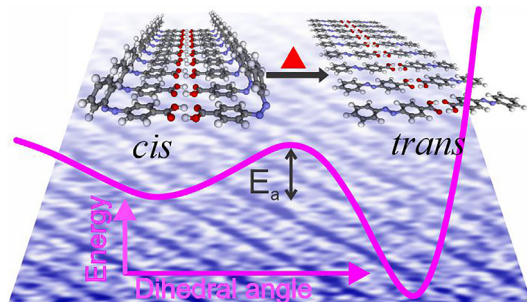
20817



### Gold nanoparticles combined with ultrafine TiO<sub>2</sub> layer: a reliable probe for Raman thermometry

Amine Khitous, Céline Molinaro,\* Anna Rumyantseva, Serguei Kochtcheev, Pierre-Michel Adam, Renaud Bachelot and Olivier Soppera\*

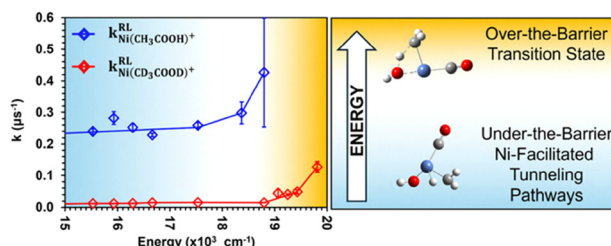
20828



### Revealing the activation barrier for the on-surface thermal-induced *cis* $\rightarrow$ *trans* isomerization of azobenzene derivatives

Hariom Birla, Thomas Halbritter, Alexander Heckel and Thiruvancheril G. Gopakumar\*

20838



### Quantum tunneling dynamics in the Ni<sup>+</sup>-mediated C–H activation of acetic acid

Gabriele Pinto, Hamed Barzinmehr, Simon U. Okafor, William Smith, Michael Brdecka, Katie L. Benjamin, Michael Gutierrez and Darrin J. Bellert\*

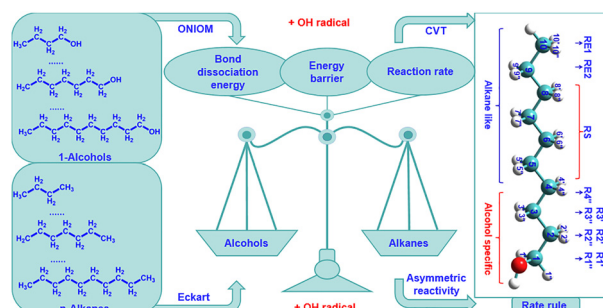


## RESEARCH PAPERS

20854

## Kinetics and general reaction rule for hydrogen atom abstraction reactions from C4–C10 alcohols by a hydroxyl radical

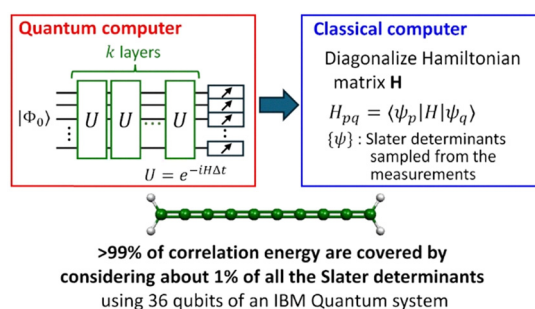
Ying Huo, Yachao Chang,\* Ming Jia\* and Lili Ye



20869

## Hamiltonian simulation-based quantum-selected configuration interaction for large-scale electronic structure calculations with a quantum computer

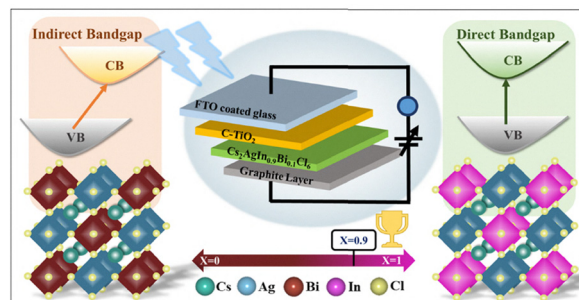
Kenji Sugisaki,\* Shu Kanno, Toshinari Itoko, Rei Sakuma and Naoki Yamamoto



20885

Exploring Cs<sub>2</sub>AgIn<sub>x</sub>Bi<sub>1-x</sub>Cl<sub>6</sub> double perovskites for optoelectronics: insights from theoretical and photophysical approaches

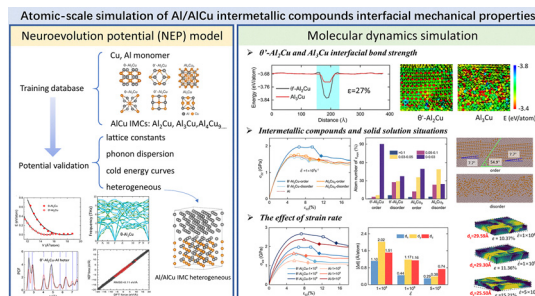
Swati N. Rahane, Ganesh K. Rahane, Yogesh Jadhav, Mamta P. Nasane, Henry I. Eya, Deepak Kalleshappa, K. Hareesh, Jayant Pawar, Sandesh R. Jadkar\* and Nelson Y. Dzade\*



20901

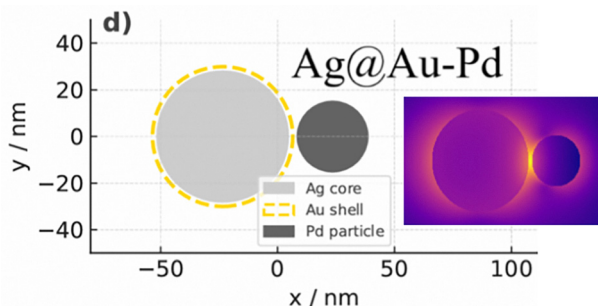
## Atomic-scale simulations of the interfacial mechanical properties of Al/AlCu intermetallic compounds

Feng-ning Xue, Zhi-qiang Hu, Yong-Chao Wu, Wei-Dong Wu, Jian-Li Shao\* and Pei Wang\*



## RESEARCH PAPERS

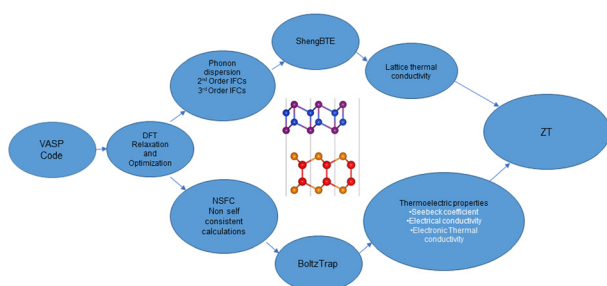
20915



## Hot carrier generation, optical chirality, and Raman enhancement in heterostructures

Mufasila Mumthaz Muhammed and Junais Habeeb Mokkaath\*

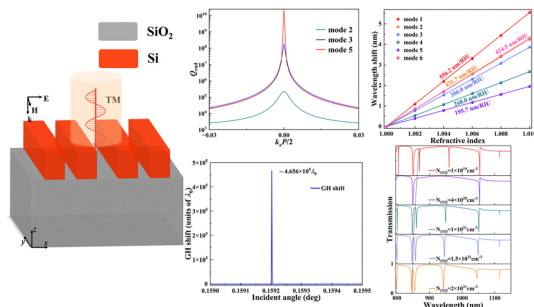
20925



## First principles study of high thermoelectric performance of two-dimensional CuI/GaTe heterostructures

Nasir Shehzad, Ismail Shahid, Shahzad Saeed, Jun Luo, Waheed-Ur-Rehman and Meng-Qiu Cai\*

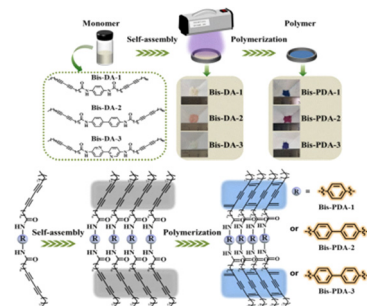
20934



## Dynamically tunable bound states in the continuum metasurfaces with simultaneous ultrahigh-Q and multi-resonance tunability

Yuanwen Deng, Boxun Li,\* Lili Zeng,\* Genxiang Zhong, Zhengchao Ma, Yang Fan, Haiqing Xu and Zhengzheng Shao

20944



## Symmetric bis-polyacetylene linked with aromatic amides targeting medium-high temperature thermal monitoring

Chunyu Song, Xuan Zhang, Chenglong Qiu and Yong Yang\*

