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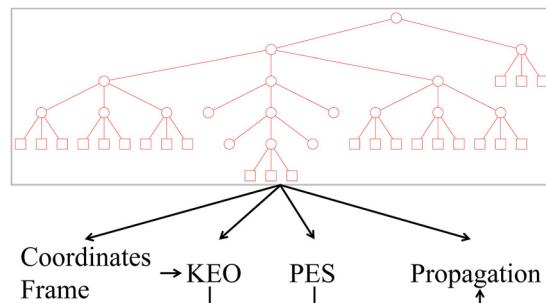
See Taro Udagawa
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PERSPECTIVE

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

Xingyu Zhang and Qingyong Meng*

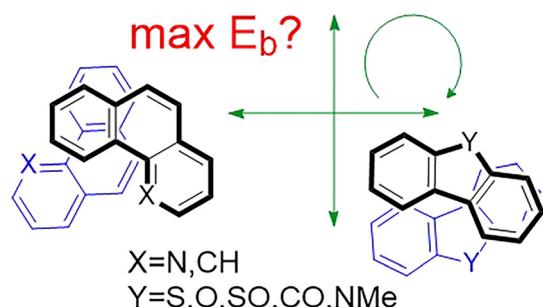


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Jessica J. Ortlieb, Nathanael J. King and Alex Brown*



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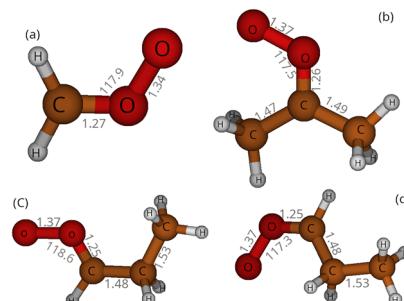
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UV photodissociation and population dynamics of some important Criegee intermediates

Behnam Nikoobakht, Maximilian F. S. J. Menger and
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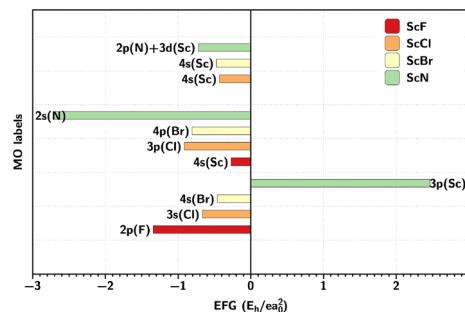


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Nuclear electric quadrupole moment of ^{45}Sc : reconfirmation and extension to diatomic ScN

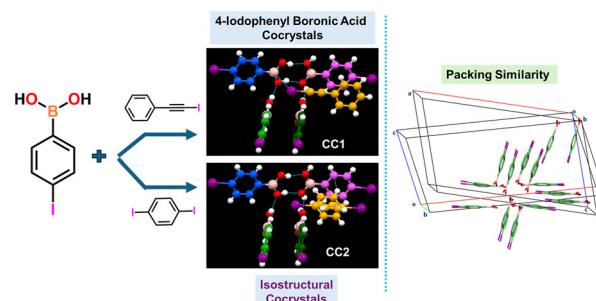
Jean-Pierre Dognon* and Pekka Pyykkö*



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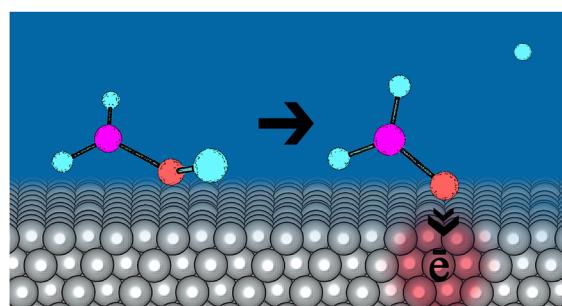
Koushik Mandal, Ajay Suresh and Deepak Chopra*



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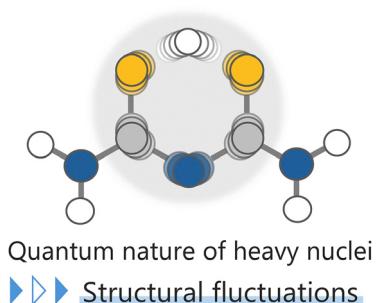
Computational investigation of charge transfer from hydroxymethyl radicals to metal surfaces suspended in water

Basil Raju Karimadom, Dan Meyerstein, Amir Mizrahi and Hava Kornweitz*



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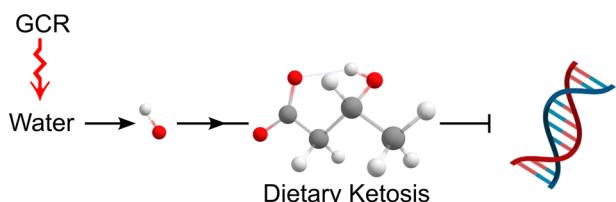
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Nuclear quantum effects on intramolecular hydrogen bonds and backbone structures in biuret analogues

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

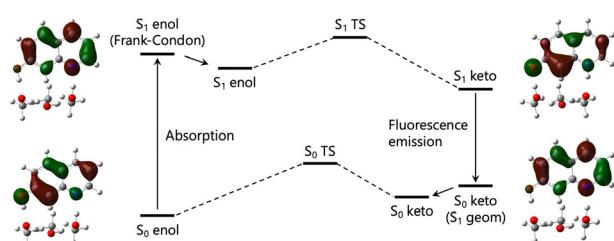
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Peter A. C. McPherson,* Ruaidhrí MacDonnell and Ben M. Johnston

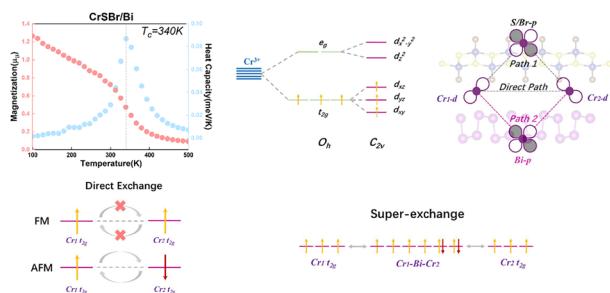
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Enhanced Curie temperature of ferromagnetic CrSBr by interfacial coupling with elemental two-dimensional ferroelectrics: triggering a new p-d super-exchange coupling path

Xiaotong Zhou and Baozeng Zhou*

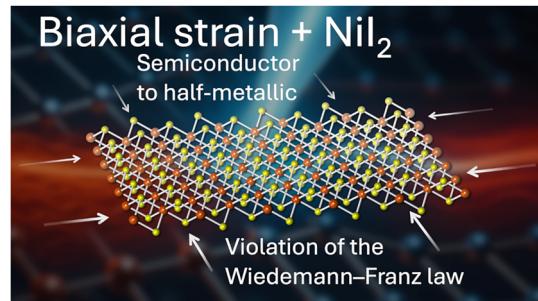


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Strain-induced half-metallicity and giant Wiedemann–Franz violation in monolayer NiI_2

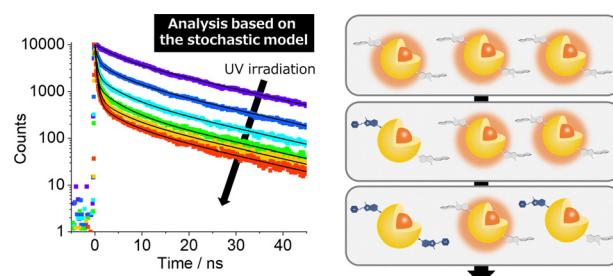
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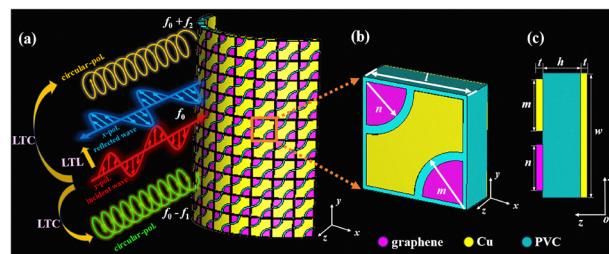
Sho Shishido, Moe Yamamoto, Daichi Eguchi* and Naoto Tamai*



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A flexible linear circular bipolarization conversion metasurface based on graphene

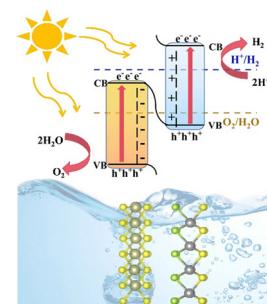
Changfeng Fu, Yu Zhu, Bo Yang, Mingzhu Ma, Mengge Lv, Shaohua Dong and Lianfu Han*



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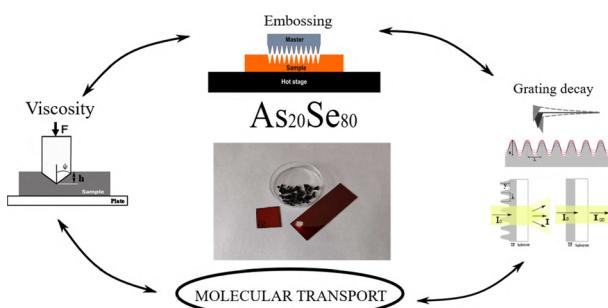
Design of Z-scheme WS₂–XS₂ (X = Zr and Hf) heterostructures as photocatalysts for efficient solar water splitting

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



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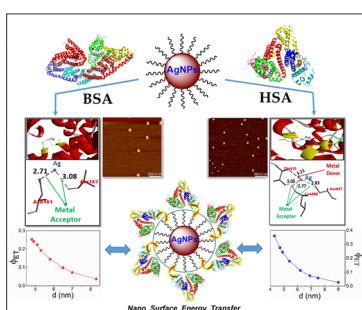
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Surface kinetics and viscosity in amorphous $\text{As}_{20}\text{Se}_{80}$: a comparative study of bulk and thin films prepared by thermal evaporation and spin-coating

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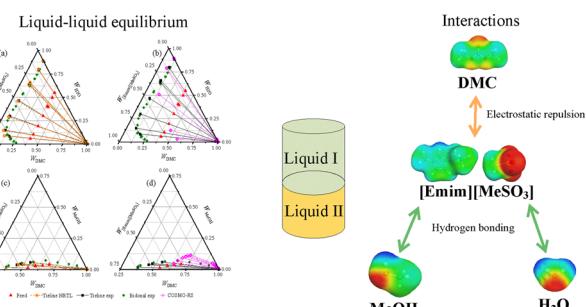
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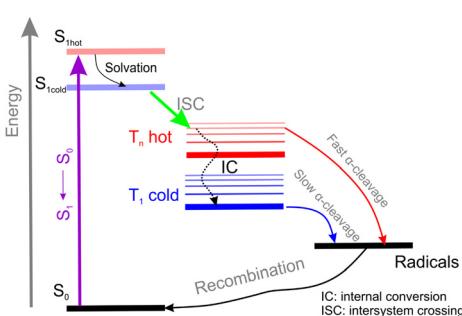
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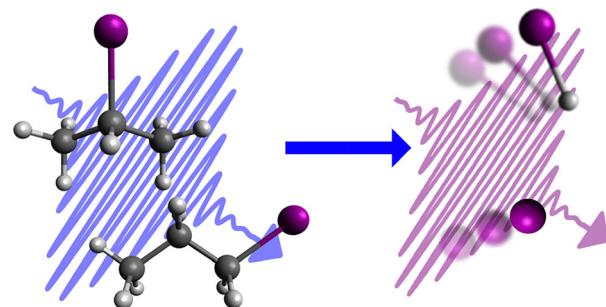


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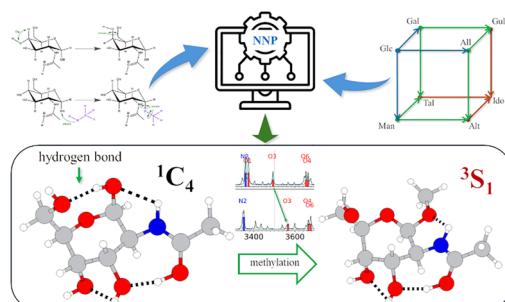
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Conformational analysis of protonated *N*-acetyl hexosamines: unexpected methylation effects from first-principles and machine learning

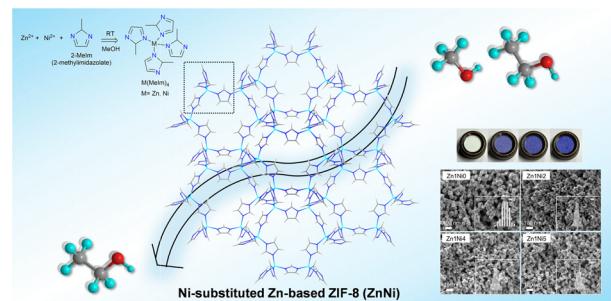
Kenee Kaiser Suyo Custodio,* Truc Quyen Vo Thi, Huu Trong Phan, Pei Kang Tsou and Jer-Lai Kuo*



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

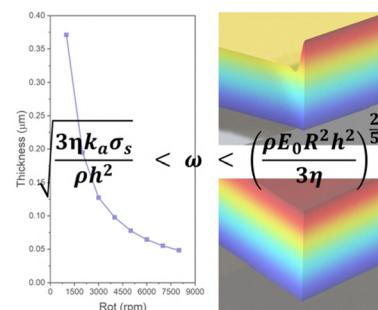
Panyapat Ponchai, Kanyaporn Adpakpang, Yollada Inchongkol, Kajjana Boonpalit, Suttipong Wannapaiboon and Sareeya Bureekaew*



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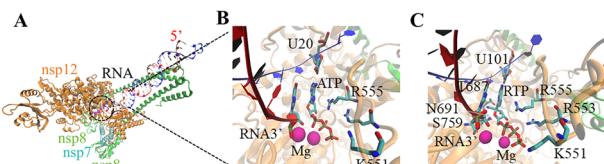
Theoretical design of critical spin speed and the process window for spin-coated self-assembled monolayers

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



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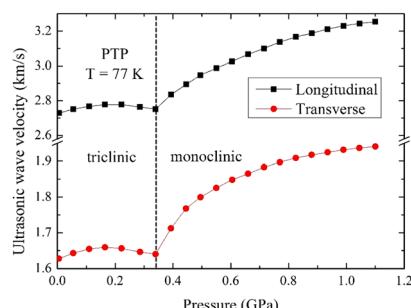
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The fidelity control of nucleotide selectivity in SARS-CoV-2 RdRp through amino acid mutations via molecular dynamics simulations

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

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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

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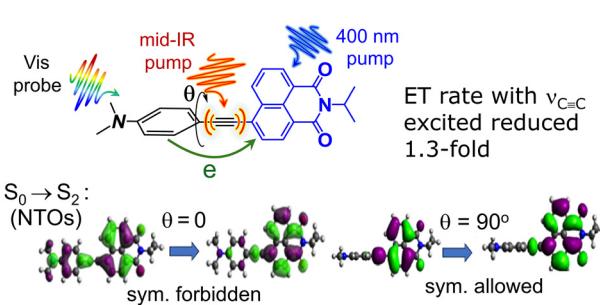
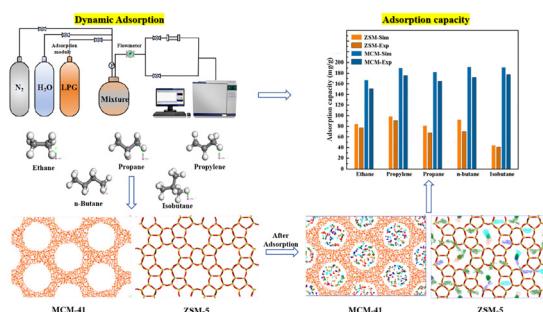


Photo-induced electron transfer dynamics and its mid-IR modulation of an ethyne bridged donor–acceptor complex

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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*

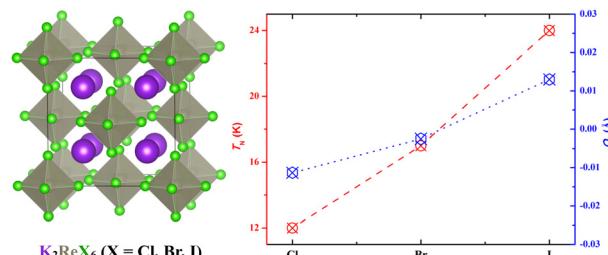


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Magnetic properties and spin–orbit coupling-driven Jahn–Teller distortions in K_2ReX_6 ($X = Cl, Br$ and I) with a half-filled $5d\text{-}t_{2g}^3$ shell

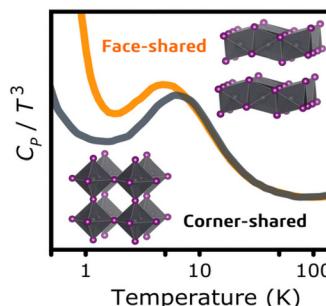
Yixuan Du, Yaoyao Hao, Xianfeng Hao,* Yongchao Jia, Keju Sun and Yuanhui Xu*



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

Ana Arauzo,* Pelayo Marin-Villa, Kacper Drużbicki, María Concepción Sánchez and Félix Fernández-Alonso*

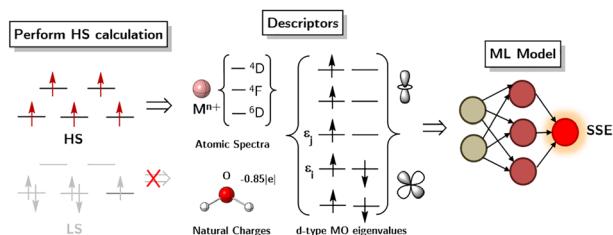


Metal Halide Perovskites
Thermophysical Fingerprints of Disorder

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

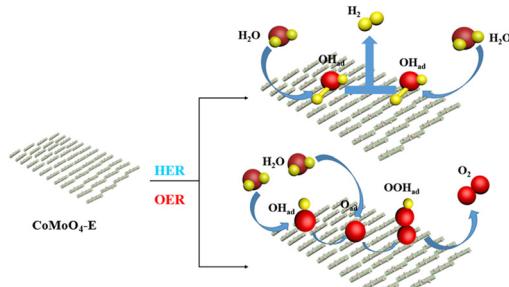
Anuj Kumar Ray, Sandeep Nagar, Girish Varma,* U. Deva Priyakumar and Ankan Paul*



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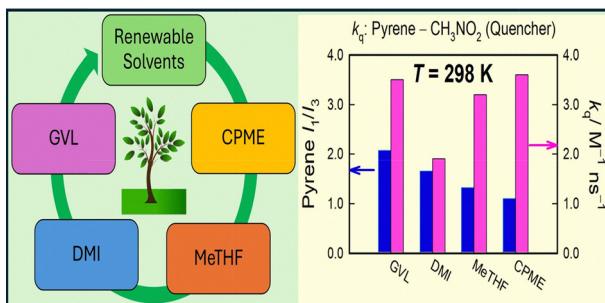
Hydroxyl-regulated $CoMoO_4$ nanotubes as an efficient bifunctional electrocatalyst for the hydrogen/oxygen evolution reaction

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*



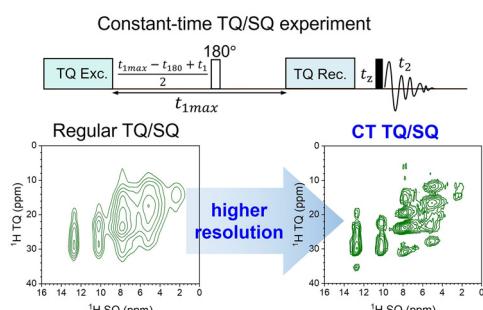
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**Investigation of solute solvation within renewable solvents via pyrene fluorescence**

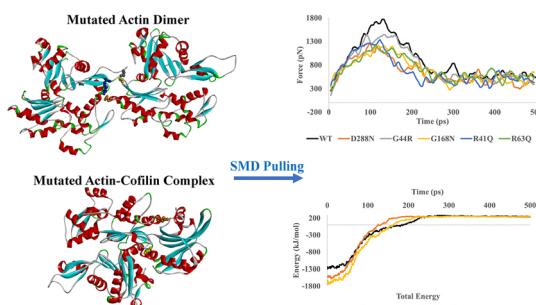
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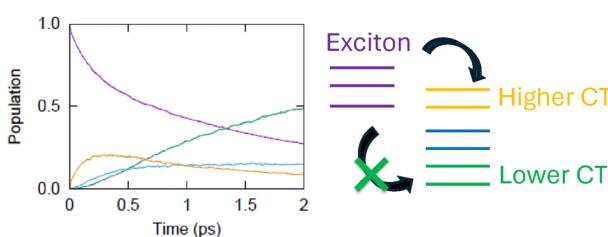
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**Exciton dissociation pathways in donor/acceptor blends studied by the wave packet dynamics approach**

Takatoshi Fujita* and Misa Nozaki

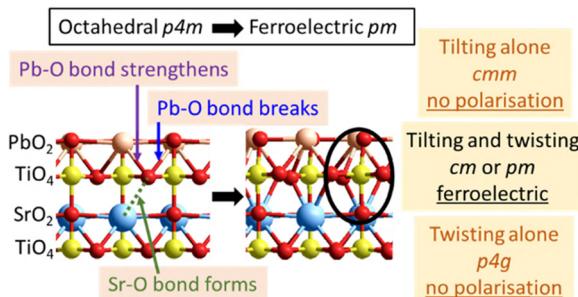


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Chemical control of polymorphism and ferroelectricity in PbTiO_3 and SrTiO_3 monolayers and bilayers

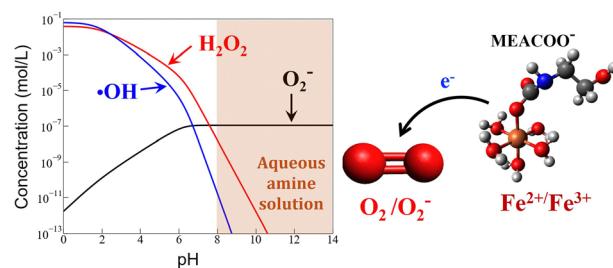
Shaowen Xu, Jeffrey R. Reimers,* Fanhao Jia and Wei Ren*



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

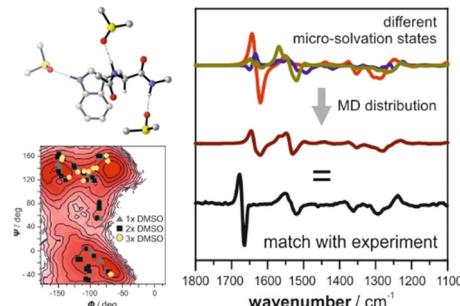
Dipam Patel, Jiwon Yu and Gyeong S. Hwang*



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

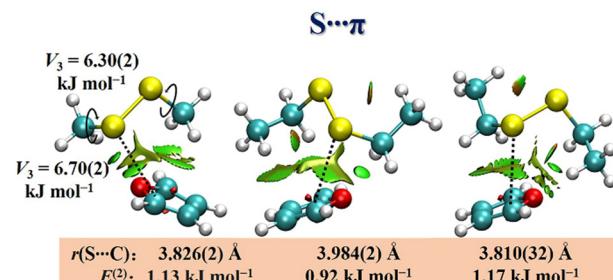
Dilber Tan, Veronika Stoianova and Christian Merten*



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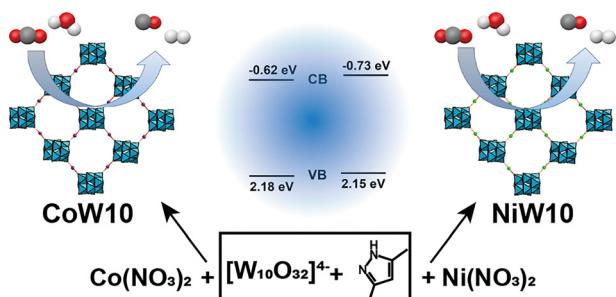
Unraveling the S–S···π interactions in furan–disulfide heterodimers: insights from microwave spectroscopy and *ab initio* computations

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



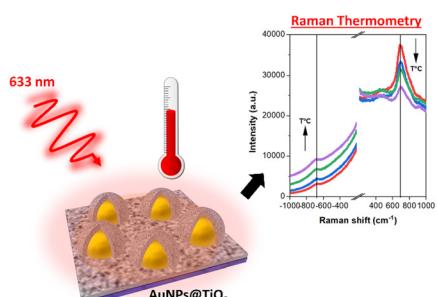
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**Visible-light driven photoreduction of carbon dioxide to syngas with decatungstate-based metal–organic frameworks**

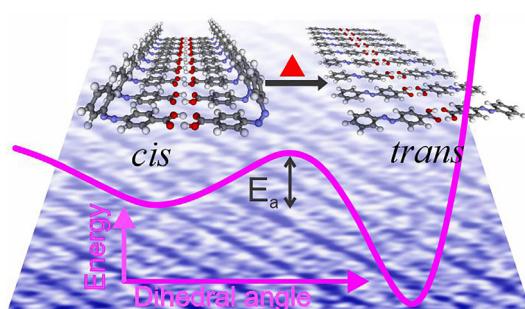
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**Gold nanoparticles combined with ultrafine TiO_2 layer: a reliable probe for Raman thermometry**

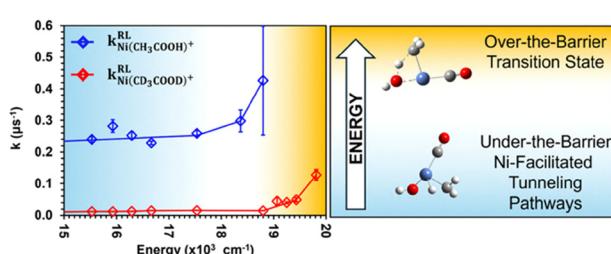
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Gabriele Pinto, Hamed Barzinmehr, Simon U. Okafor, William Smith, Michael Brdecka, Katie L. Benjamin, Michael Gutierrez and Darrin J. Bellert*

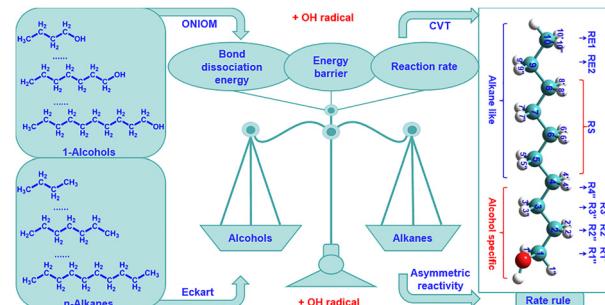


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Kinetics and general reaction rule for hydrogen atom abstraction reactions from C4–C10 alcohols by a hydroxyl radical

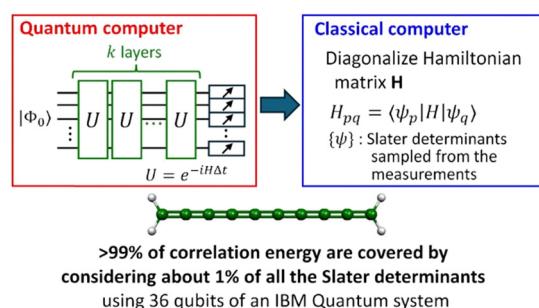
Ying Huo, Yachao Chang,* Ming Jia* and Lili Ye



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

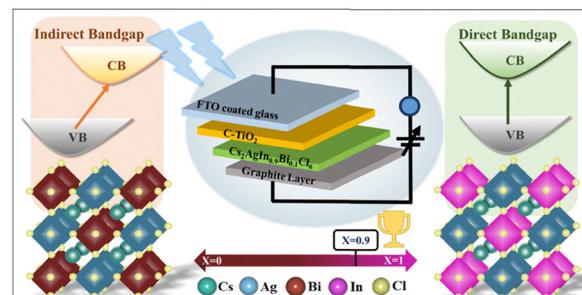
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Exploring $\text{Cs}_2\text{AgIn}_x\text{Bi}_{1-x}\text{Cl}_6$ double perovskites for optoelectronics: insights from theoretical and photophysical approaches

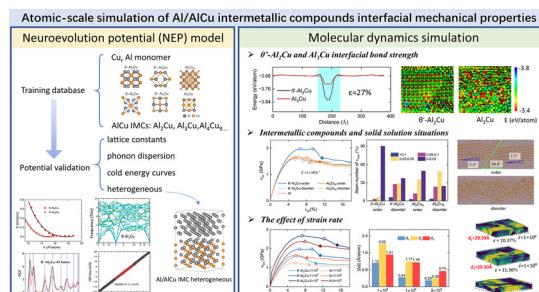
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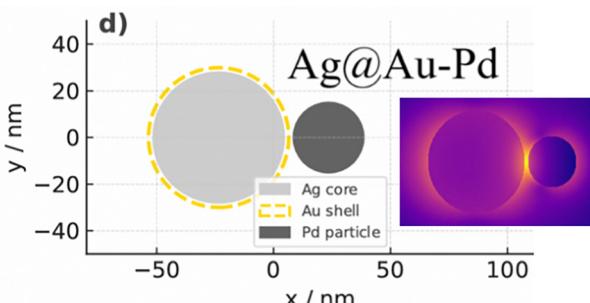
Atomic-scale simulations of the interfacial mechanical properties of Al/AlCu intermetallic compounds

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



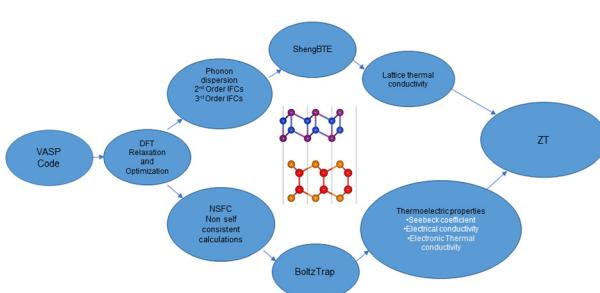
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**Hot carrier generation, optical chirality, and Raman enhancement in heterostructures**

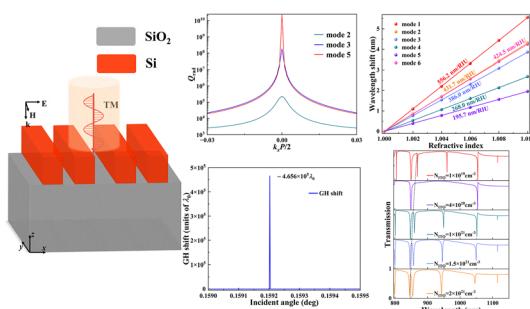
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**First principles study of high thermoelectric performance of two-dimensional CuI/GaTe heterostructures**

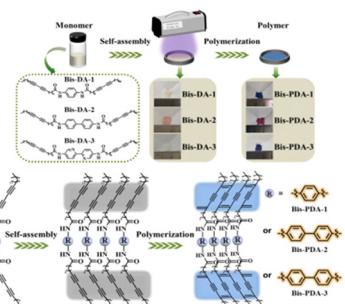
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Yuanwen Deng, Boxun Li,* Lili Zeng,* Genxiang Zhong, Zhengchao Ma, Yang Fan, Haiqing Xu and Zhengzheng Shao

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

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

