

# 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(10) 4979–5406 (2025)



### Cover

See Peter Vöhringer *et al.*, pp. 5012–5023. Image reproduced by permission of Peter Vöhringer from *Phys. Chem. Chem. Phys.*, 2025, 27, 5012.



### Inside cover

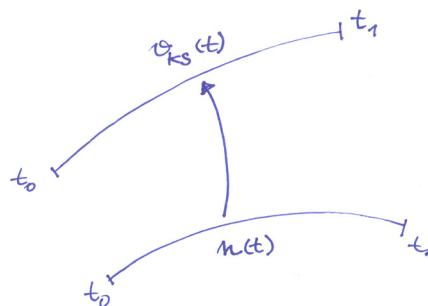
See Takaya Fujisaki, Yusuke Shiratori *et al.*, pp. 5024–5036. Image reproduced by permission of Hibiki Asahori from *Phys. Chem. Chem. Phys.*, 2025, 27, 5024.

## TUTORIAL REVIEW

4992

### Review of the foundations of time-dependent density-functional theory (TDDFT)

J. Schirmer



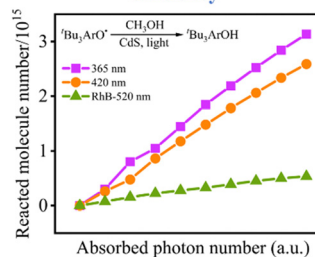
## COMMUNICATION

5006

### Anti-Kasha's rule for semiconductor photocatalytic reactions: the wavelength dependence of quantum efficiency

Yuhan Lin,\* Yi He, Qiang Wang, Jie Feng, Yue Hou and Chuanyi Wang\*

#### Wavelength-dependent quantum efficiency



# Industrial Chemistry & Materials



Focus on industrial chemistry  
Advance material innovations  
Highlight interdisciplinary feature



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)

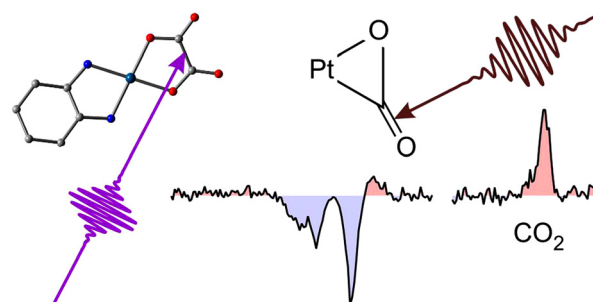


## RESEARCH PAPERS

5012

### Photoinduced formation of a platina- $\alpha$ -lactone – a carbon dioxide complex of platinum. Insights from femtosecond mid-infrared spectroscopy

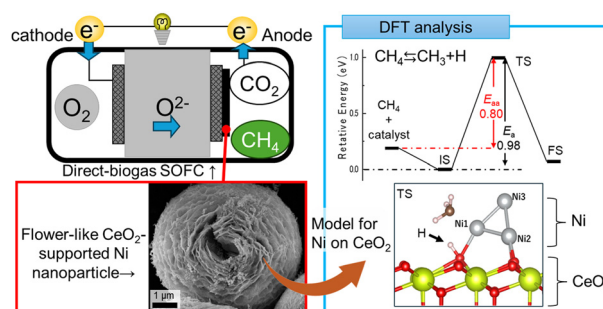
Markus Bauer, Raphaela Post, Luis I. Domenianni and Peter Vöhringer\*



5024

### Investigating Ni nanoparticles on CeO<sub>2</sub> for methane dissociation: a comparative study of theoretical calculations and experimental insights

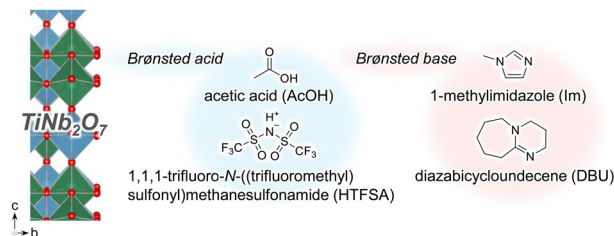
Takaya Fujisaki,\* Yuta Tsuji, Phuc Hoan Tu, Tin Chanh Duc Doan, David S. Rivera Rocabado, Aleksandar Tsekov Staykov, Keiji Yashiro and Yusuke Shiratori\*



5037

### Electrochemical protonation/deprotonation of TiNb<sub>2</sub>O<sub>7</sub> in protic ionic liquids

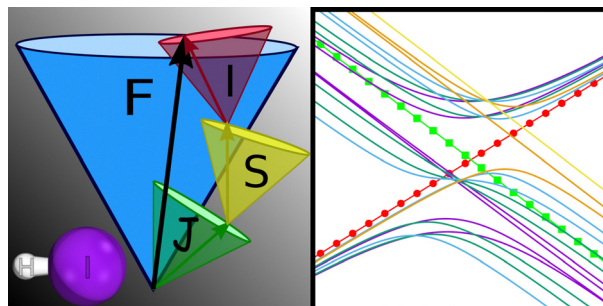
Masahiro Shimizu,\* Takuya Kawai, Tomonori Ichikawa and Susumu Arai



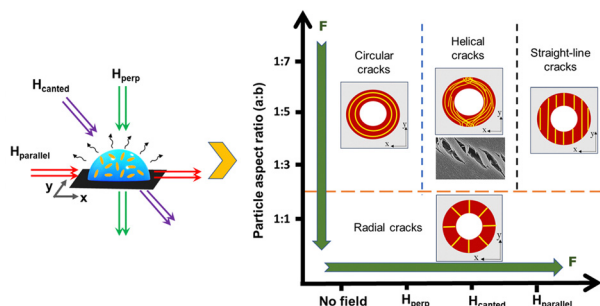
5043

### Accurate incorporation of hyperfine coupling in diabatic potential models using the effective relativistic coupling by asymptotic representation approach

Maik Vossel, Iordanis Tsakontsis, Nicole Weike and Wolfgang Eisfeld\*



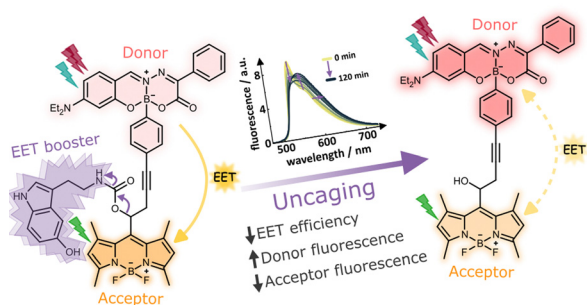
5056



### Crack control in dried ferro-colloidal droplets: effect of particle aspect-ratio and magnetic field orientations

Deeksha Rani\* and Subhendu Sarkar

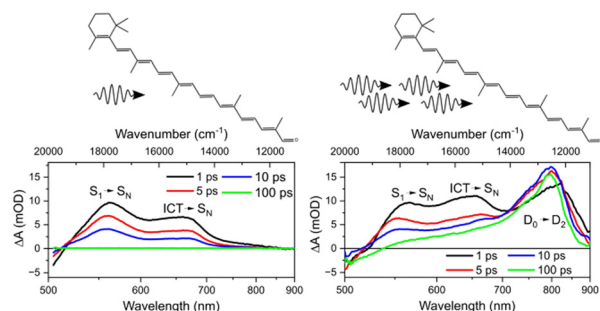
5064



### Energy transfer booster: how a leaving group controls the excited state pathway within a caging BASHY–BODIPY dyad

Yagmur Aydogan-Sun, Maximiliane Horz, Rebekka Weber, Myron Heinz, Markus Braun, Alexander Heckel,\* Irene Burghardt\* and Josef Wachtveitl\*

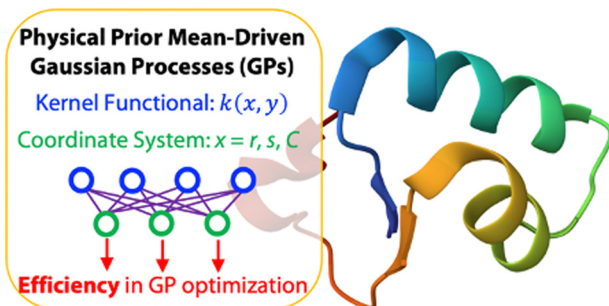
5080



### Carotenoid radical formation after multi-photon excitation of 8'-apo- $\beta$ -carotenal

Václav Šebelík, Valentyna Kuznetsova, Ivana Šimová and Tomáš Polívka\*

5087



### First-principle oligopeptide structural optimization with physical prior mean-driven Gaussian processes: a test of synergistic impacts of the kernel functional and coordinate system

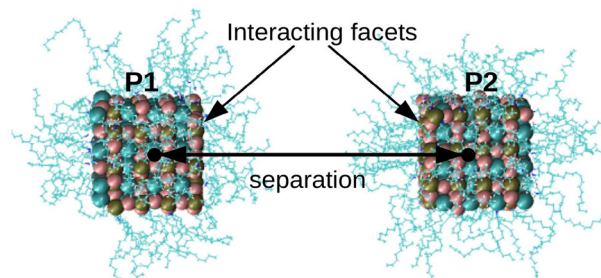
Yibo Chang, Chong Teng and Junwei Lucas Bao\*



5098

### Ligand-mediated interaction in a dispersion of lead-halide perovskite nanocubes: implications on directed structures in equilibrium

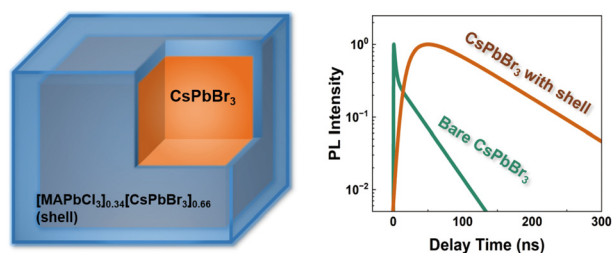
Avik Sasmal,\* Edwine Tendong,\* Tanusri Saha-Dasgupta and Jaydeb Chakrabarti



5109

### Carrier recombination dynamics in [MAPbCl<sub>3</sub>]<sub>x</sub>[CsPbBr<sub>3</sub>]<sub>1-x</sub> shell-passivated CsPbBr<sub>3</sub> single crystals

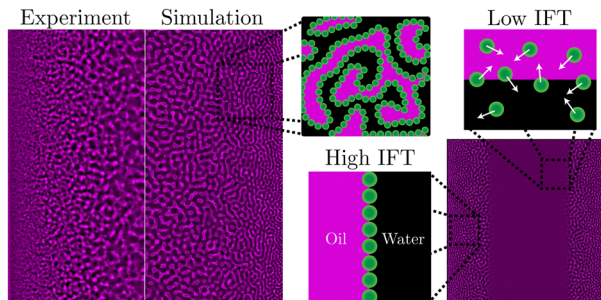
Zheng Zou, Zijie Xiao, Wenxin Dong, Wei Dang,\* Shusheng Pan, Xiaojun Su and Wei Zhang\*



5117

### Analysis of bijel formation dynamics during solvent transfer-induced phase separation using phase-field simulations

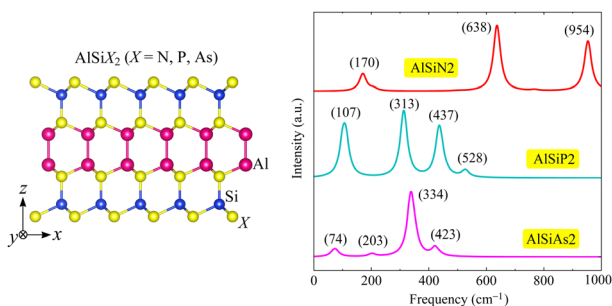
Jesse M. Steenhoff\* and Martin F. Haase\*



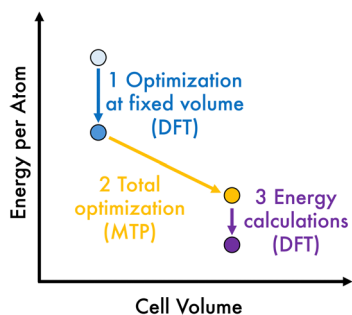
5131

### Two-dimensional piezoelectric AlSiX<sub>2</sub> (X = N, P, As) semiconductors with Raman activity, favorable band-gap, and high carrier mobility based on first-principles calculations

Tuan V. Vu, Nguyen N. Hieu, Nguyen T. Hiep, Thuat T. Trinh, A. I. Kartamyshev and Huynh V. Phuc\*



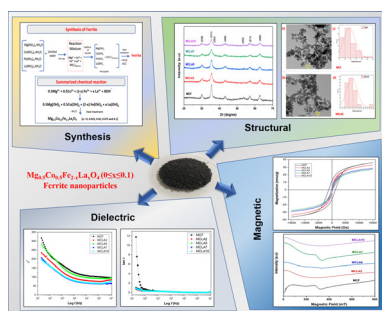
5141



### Accelerating structure prediction of molecular crystals using actively trained moment tensor potential

Nikita Rybin,\* Ivan S. Novikov and Alexander Shapeev

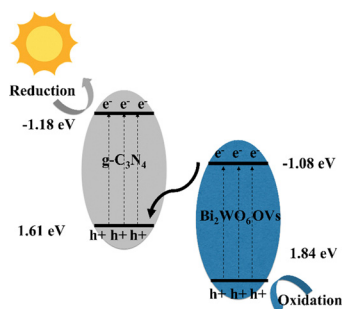
5149



### Impact of La<sup>3+</sup> doping on the structural, magnetic, and dielectric properties of Mg–Co ferrites for high-frequency applications

Rohit, Vasundhara Madaan, Richa Jain, Sourabh Sharma, Vinita Bhankar, Ashok Kumar\* and Krishan Kumar\*

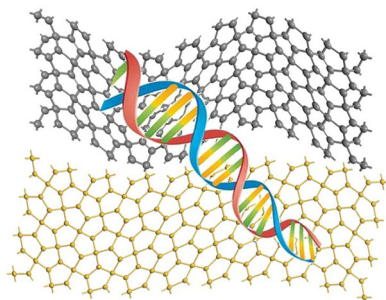
5163



### Z-type heterojunction degradation of tetracycline by 2D g-C<sub>3</sub>N<sub>4</sub> with 3D oxygen vacancy Bi<sub>2</sub>WO<sub>6</sub>

Xiao Kang, Xiangyan Li, Abulikemu Abulizi, Mihiriguli Abulimiti, Nuerla Ailijiang and Anwar Mamat\*

5172



### In-depth electronic behavior of pentagraphene and pentagonal silicene sheets for DNA nucleobase detection: implications for genetic biomarker sensing

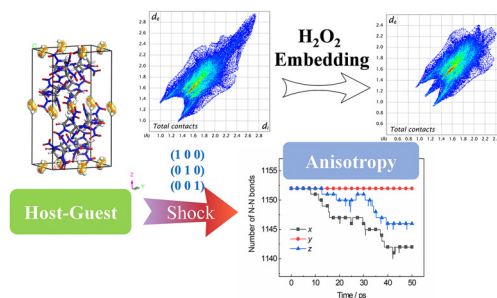
Arzoo Hassan, Andleeb Mehmood, Umer Younis and Xiaoqing Tian\*



5186

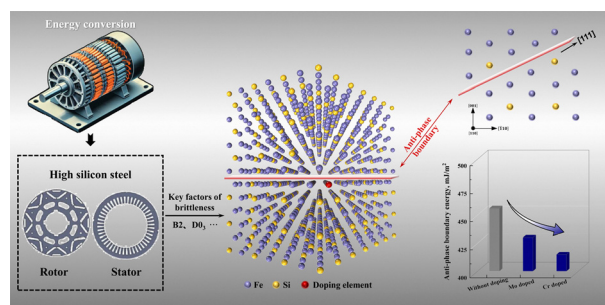
### Anisotropic initial reaction mechanism and sensitivity characterization of the host-guest structure CL-20/H<sub>2</sub>O<sub>2</sub> under shock loading

Yu Sha and Xiaobing Zhang\*



5198

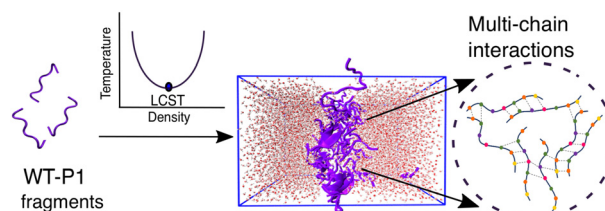
### Effects of doping on anti-phase boundaries and the magnetic properties of the D0<sub>3</sub> structure in high silicon steel: first-principles insights

Meng Sun, Linxian Li, Hongyu Song, Shuai Tang,\*  
Qing Peng,\* Guichang Shen, Tianwei Xie,  
Fengliang Tan and Zhenyu Liu

5206

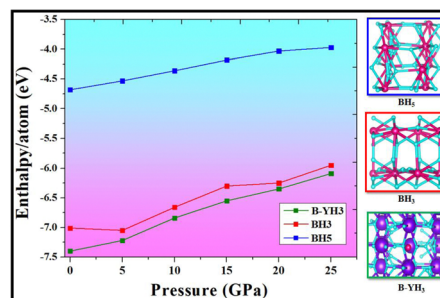
### Insight into the thermo-responsive phase behavior of the P1 domain of $\alpha$ -synuclein using atomistic simulations

Sanchari Chakraborty and Mithun Biswas\*

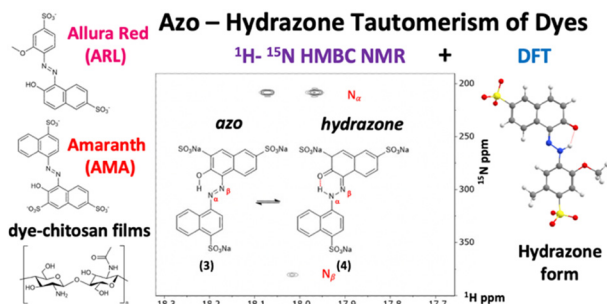


5215

### Electron doping in non-magnetic YH<sub>3</sub> leads to room temperature ferromagnetism and a flat band: insights from density functional theory

Pratap Mane, Ravi Kumar Trivedi, Parthasarathy Velusamy  
and Brahmananda Chakraborty\*

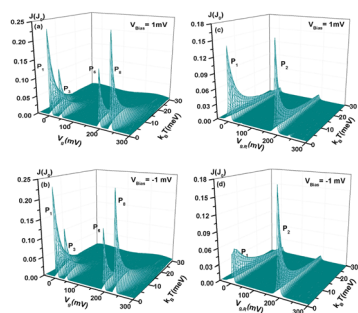
5228



### Solid state NMR and DFT studies of azo–hydrazone tautomerism in azo dyes and chitosan-dye films

Coral Hillel, Sarah Collins, Amanpreet Parihar, Ozzy Mermut, Christopher J. Barrett, William J. Pietro and Linda Reven\*

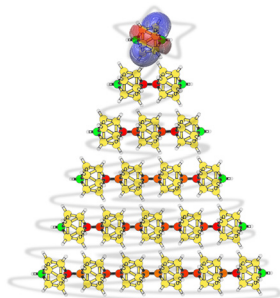
5238



### Temperature-stable tunneling current in serial double quantum dots: insights from nonequilibrium green functions and Pauli spin blockade

David M. T. Kuo

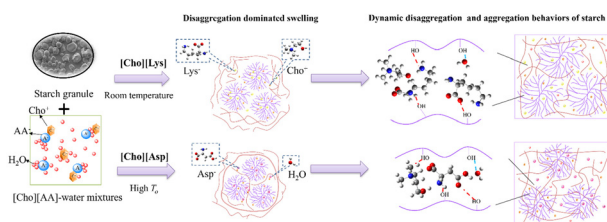
5249



### Aromatic trails: persistence and interplay between linked spherical aromatic dicarboranes in dimer to hexamer linear arrays

Alvaro Muñoz-Castro

5256



### Dissociation and aggregation behaviors of starch in choline amino acid ionic liquid solvents: the anion structure effect

Jin Chen, Xixi Zeng and Ling Chen\*

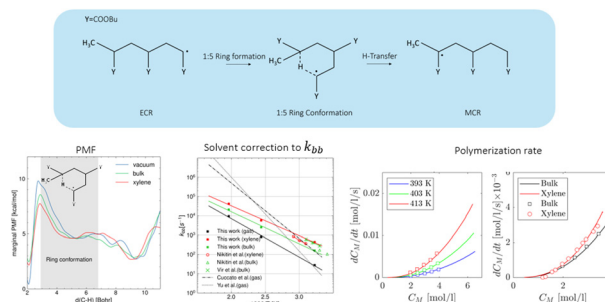


## RESEARCH PAPERS

5271

### First principles assessment of solvent induced cage effects on intramolecular hydrogen transfer in the free radical polymerization of acrylates

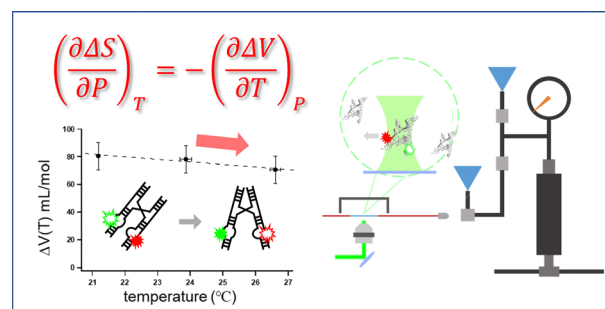
Francesco Serse,\* Matteo Salvalaglio and Matteo Pelucchi\*



5285

### Two-dimensional (P/T) studies of secondary/tertiary conformational dynamics in nucleic acids: pressure induced melting and Maxwell relations at the single molecule level

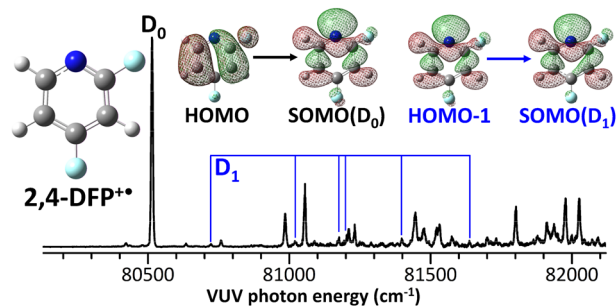
Hsuan-Lei Sung and David J. Nesbitt\*



5296

### Uncovering the role of fluorine positioning on the cationic properties of 2,4-difluoropyridine

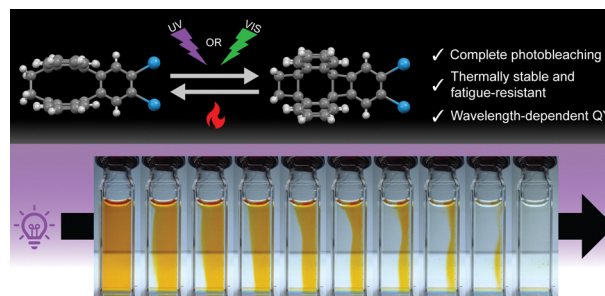
Hyojung Kim, Sung Man Park and Chan Ho Kwon\*



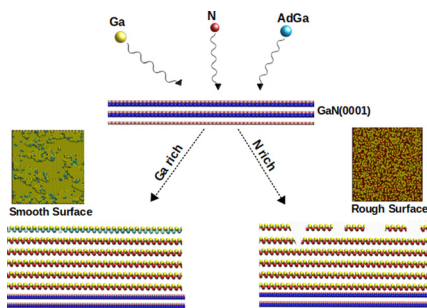
5305

### Using an aromatic linker to optimize charge-resonance states, photodimerization and reversibility in covalent anthracene dimers

Kevin Lam, Robert J. Dillon, Abel Carreras,\* Tomohiko Nishiuchi, Takashi Kubo,\* Rabih O. Al-Kaysi, David Casanova and Christopher J. Bardeen\*



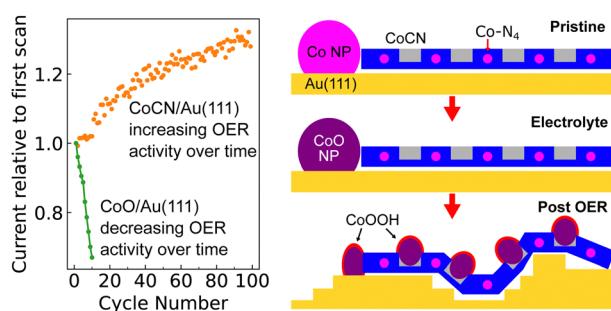
5317



### Ga adlayer model: capturing features of GaN(0001) growth from the submonolayer to the multilayer regime

Razia and Madhav Ranganathan\*

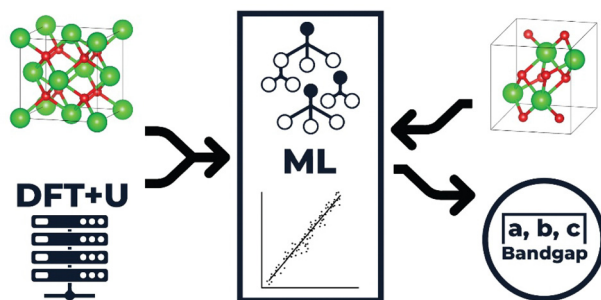
5326



### X-ray spectroscopy characterization of cobalt stabilization within a monolayer carbon nitride in the oxygen evolution reaction

Anders K. Vestergaard, Jens Jakob Gammelgaard, Zhaozong Sun, Siqi Zhao, Zheshen Li, Nina Lock, Kim Daasbjerg and Jeppe V. Lauritsen\*

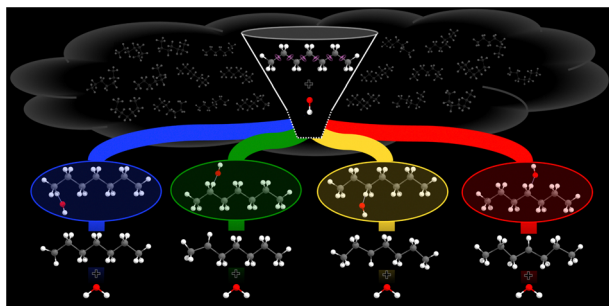
5338



### Integrating density functional theory with machine learning for enhanced band gap prediction in metal oxides

Chidozie Ezeakunne, Bipin Lamichhane and Shyam Kattel\*

5359



### Molecular conformational effects on the overall rate constant and the branching ratios of the *n*-heptane + OH reaction: an *ab initio* and variational transition state theory study

M. Belmekki, M. Monge-Palacios,\* T. Wang and S. M. Sarathy

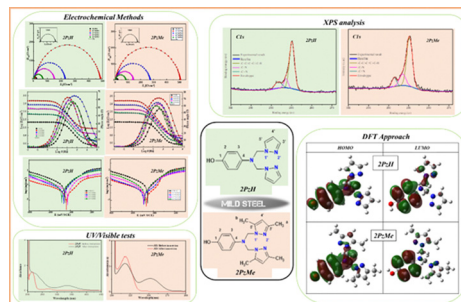


## RESEARCH PAPERS

5371

### Structural effect of bipyrazole derivatives on corrosion inhibition of carbon steel in 1 M HCl: weight loss, electrochemical measurements, XPS/SEM surface analysis, DFT and MC simulations

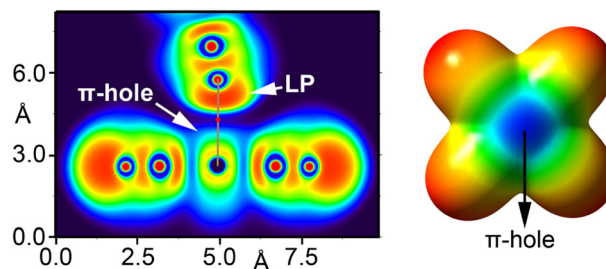
N. Setti, A. Barrahi, M. Maatallah, Y. Kaddouri, R. Touzani, B. Dikici, K. Karrouchi, Hatem A. Abuelizz, A. Zarrouk\* and A. Dafali\*



5395

### Exploring coinage bonding interactions in $[\text{Au}(\text{CN})_4]^-$ assemblies with silver and zinc complexes: a structural and theoretical study

Alessia Giordana, Emanuele Priola,\* Ghodrat Mahmoudi,\* Esmail Doustkhah, Rosa M. Gomila, Ennio Zangrando, Eliano Diana, Lorenza Operti and Antonio Frontera\*



## CORRECTION

5404

### Correction: Effects of pressure and temperature on topological electronic materials $\text{X}_2\text{Y}_3$ (X = As, Sb, Bi; Y = Se, Te) using first-principles

Le Fang, Chen Chen, Xionggang Lu\* and Wei Ren\*

