

## IN THIS ISSUE

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### Cover

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### Inside cover

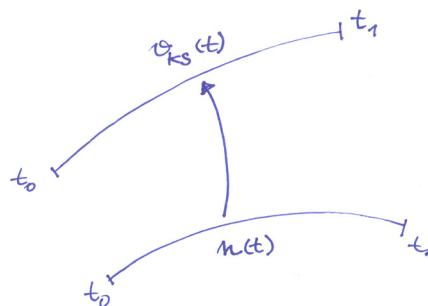
See Takaya Fujisaki, Yusuke Shiratori *et al.*, pp. 5024–5036. Image reproduced by permission of Hibiki Asahori from *Phys. Chem. Chem. Phys.*, 2025, 27, 5024.

## TUTORIAL REVIEW

4992

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

J. Schirmer



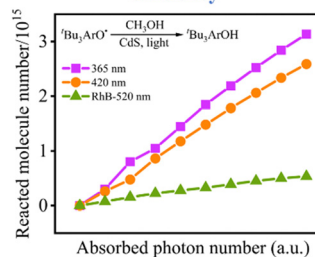
## COMMUNICATION

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



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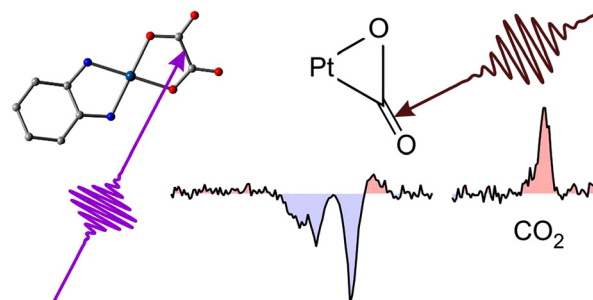


## RESEARCH PAPERS

5012

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

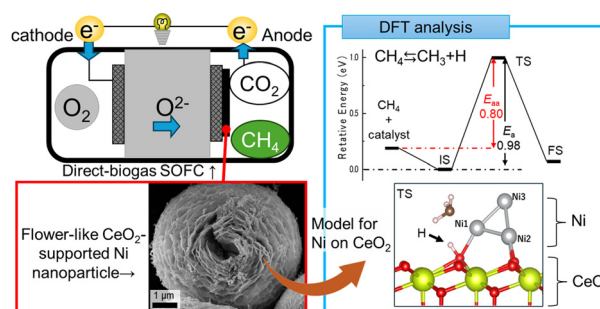
Markus Bauer, Raphaela Post, Luis I. Domenianni and Peter Vöhringer\*



5024

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

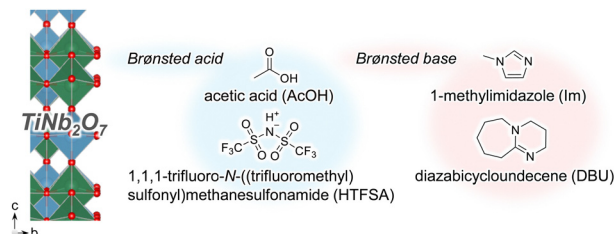
Takaya Fujisaki,\* Yuta Tsuji, Phuc Hoan Tu, Tin Chanh Duc Doan, David S. Rivera Rocabado, Aleksandar Tsekov Staykov, Keiji Yashiro and Yusuke Shiratori\*



5037

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

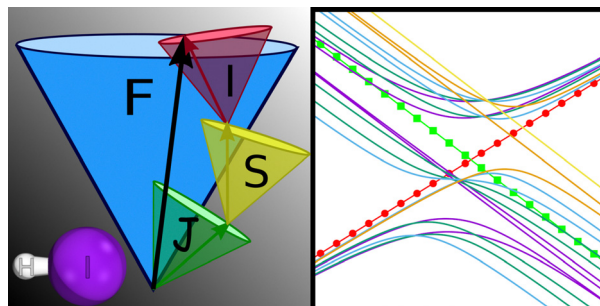
Masahiro Shimizu,\* Takuya Kawai, Tomonori Ichikawa and Susumu Arai



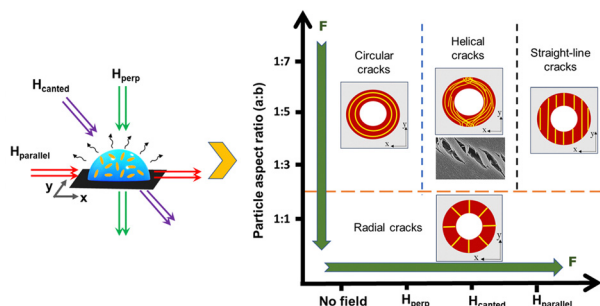
5043

### 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\*



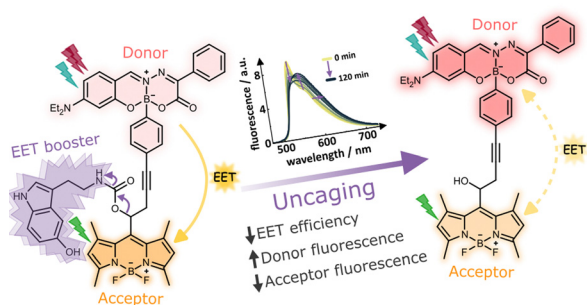
5056



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

Deeksha Rani\* and Subhendu Sarkar

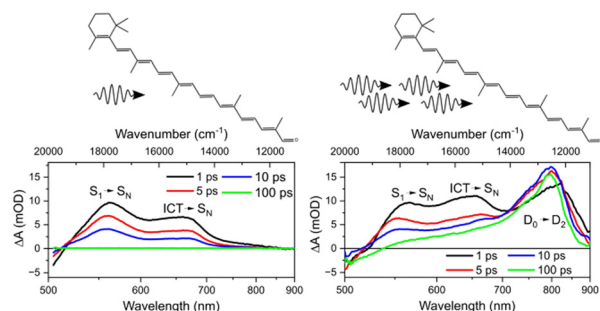
5064



### 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\*

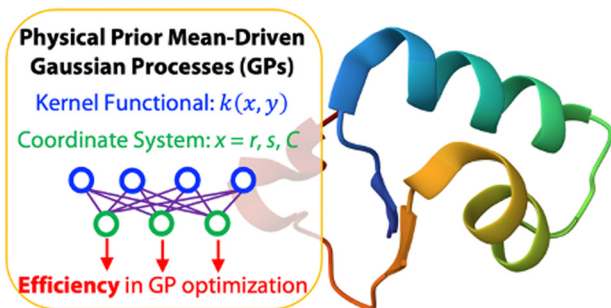
5080



### Carotenoid radical formation after multi-photon excitation of 8'-apo-β-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

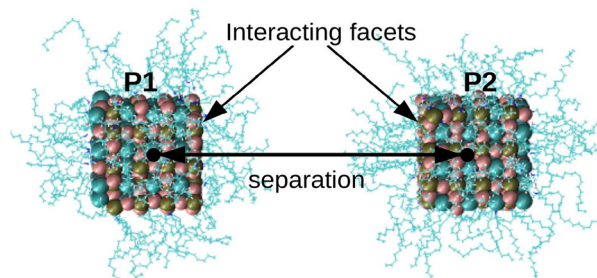
Yibo Chang, Chong Teng and Junwei Lucas Bao\*



5098

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

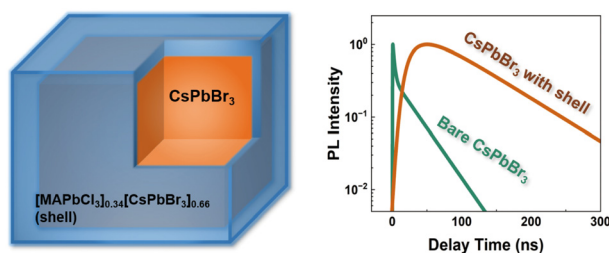
Avik Sasmal,\* Edwine Tendong,\* Tanusri Saha-Dasgupta and Jaydeb Chakrabarti



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

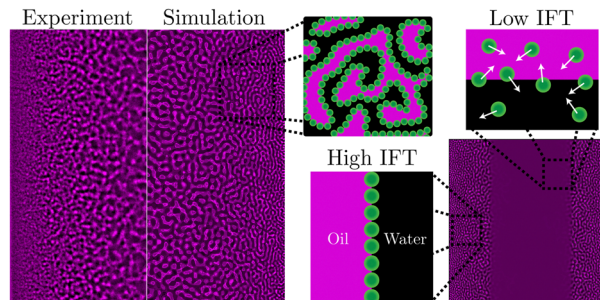
Zheng Zou, Zijie Xiao, Wenxin Dong, Wei Dang,\* Shusheng Pan, Xiaojun Su and Wei Zhang\*



5117

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

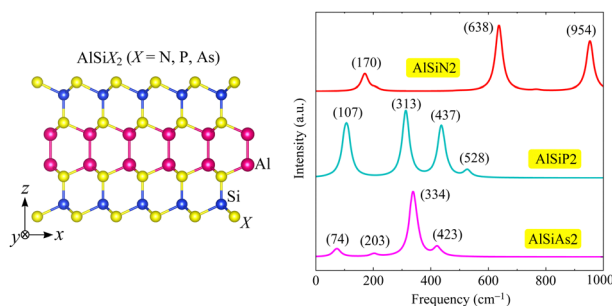
Jesse M. Steenhoff\* and Martin F. Haase\*



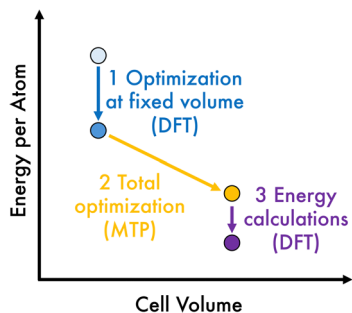
5131

### 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\*



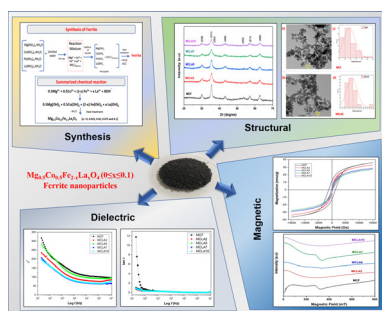
5141



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

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

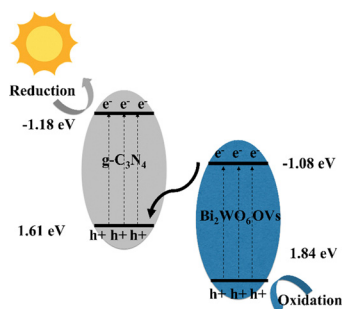
5149



### Impact of $La^{3+}$ 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\*

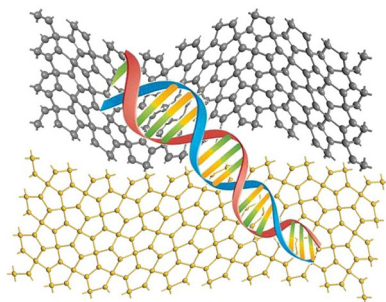
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### Z-type heterojunction degradation of tetracycline by 2D $g-C_3N_4$ with 3D oxygen vacancy $Bi_2WO_6$

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

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### 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\*

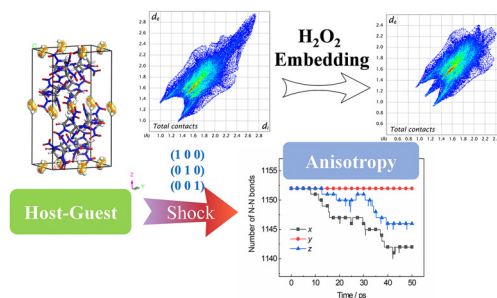


## RESEARCH PAPERS

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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

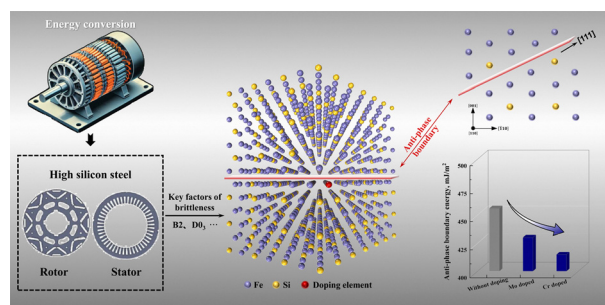
Yu Sha and Xiaobing Zhang\*



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

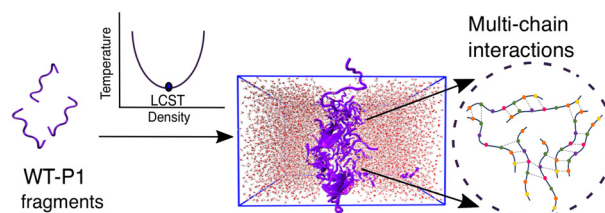
Meng Sun, Linxian Li, Hongyu Song, Shuai Tang,\* Qing Peng,\* Guichang Shen, Tianwei Xie, Fengliang Tan and Zhenyu Liu



5206

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

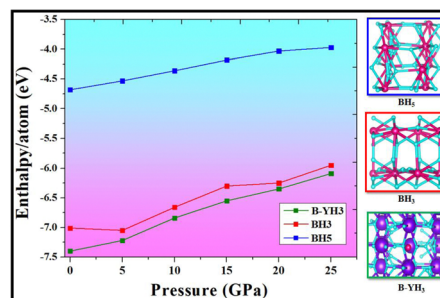
Sanchari Chakraborty and Mithun Biswas\*



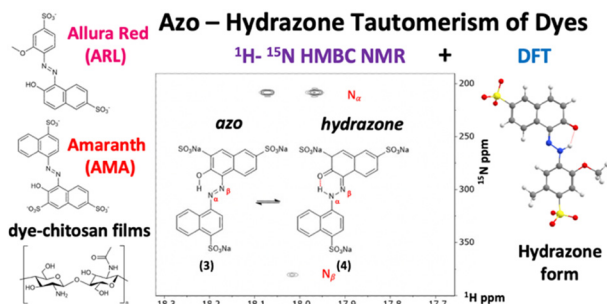
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Electron doping in non-magnetic YH<sub>3</sub> leads to room temperature ferromagnetism and a flat band: insights from density functional theory

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



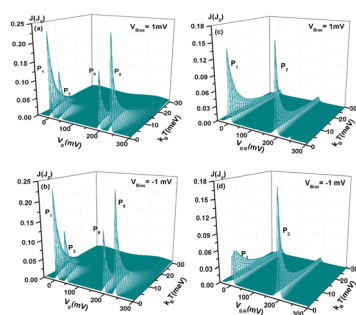
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### Solid state NMR and DFT studies of azo–hydrazone tautomerism in azo dyes and chitosan-dye films

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

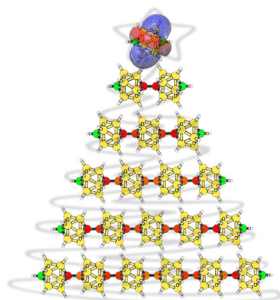
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### Temperature-stable tunneling current in serial double quantum dots: insights from nonequilibrium green functions and Pauli spin blockade

David M. T. Kuo

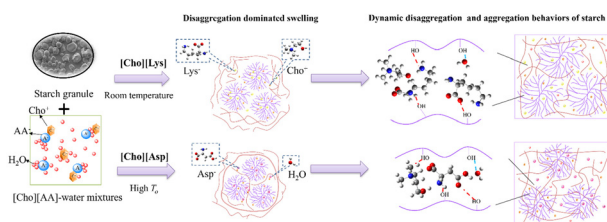
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### Aromatic trails: persistence and interplay between linked spherical aromatic dicarboranes in dimer to hexamer linear arrays

Alvaro Muñoz-Castro

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

Jin Chen, Xixi Zeng and Ling Chen\*

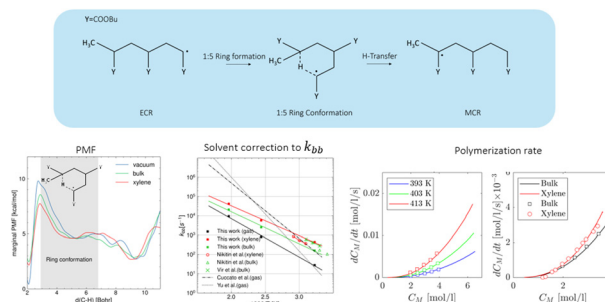


## RESEARCH PAPERS

5271

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

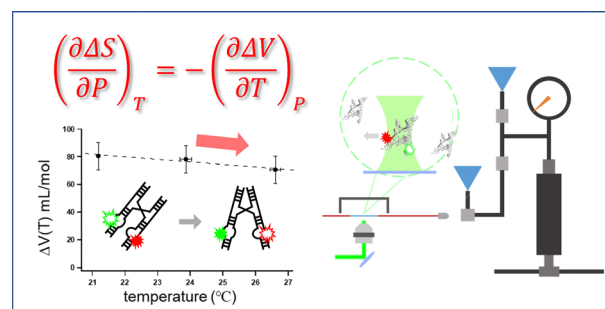
Francesco Serse,\* Matteo Salvalaglio and Matteo Pelucchi\*



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

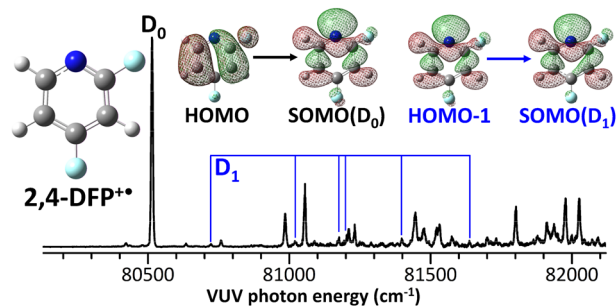
Hsuan-Lei Sung and David J. Nesbitt\*



5296

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

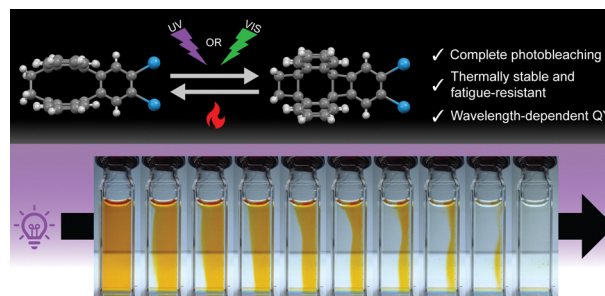
Hyojung Kim, Sung Man Park and Chan Ho Kwon\*



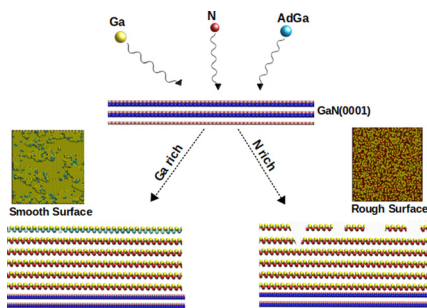
5305

### 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\*



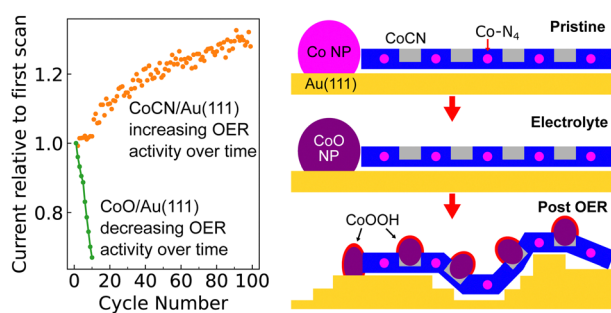
5317



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

Razia and Madhav Ranganathan\*

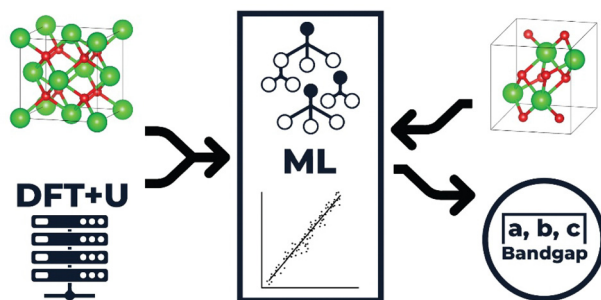
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### X-ray spectroscopy characterization of cobalt stabilization within a monolayer carbon nitride in the oxygen evolution reaction

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

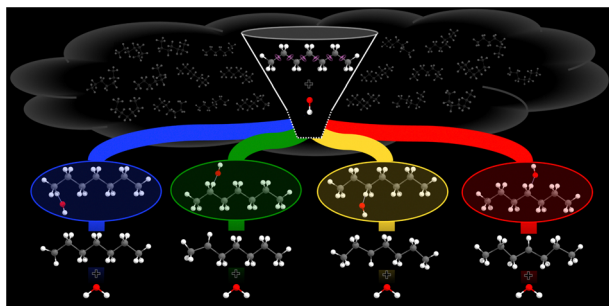
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### Integrating density functional theory with machine learning for enhanced band gap prediction in metal oxides

Chidozie Ezeakunne, Bipin Lamichhane and Shyam Kattel\*

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### 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

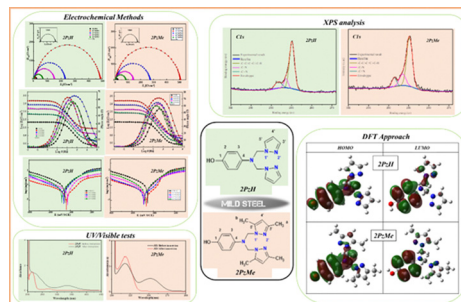


## RESEARCH PAPERS

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

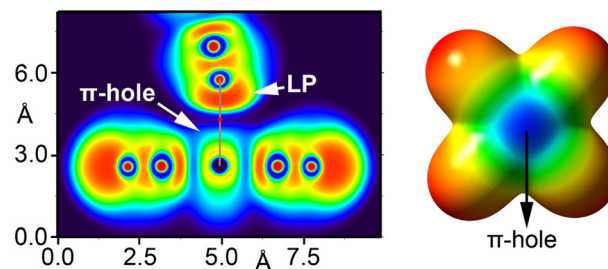
N. Setti, A. Barrahi, M. Maatallah, Y. Kaddouri, R. Touzani, B. Dikici, K. Karrouchi, Hatem A. Abuelizz, A. Zarrouk\* and A. Dafali\*



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\*

