Open Access Article. Published on 06 March 2025. Downloaded on 2/1/2026 4:03:59 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

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.

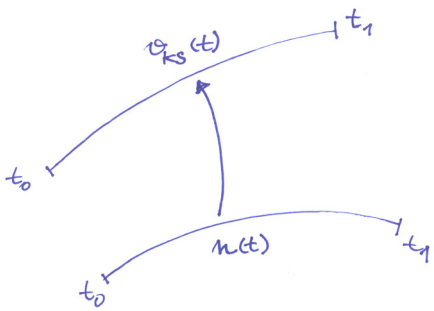
Inside cover
See Takaya Fujisaki, Yusuke Shiratori *et al.*, pp. 5024–5036. Image reproduced by permission of Hibiki Asahori from *Phys. Chem. Chem. Phys.*, 2025, **27**, 5024.

TUTORIAL REVIEW

4992

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

J. Schirmer

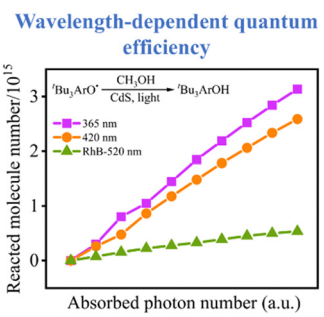


COMMUNICATION

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*



View Article Online

Industrial Chemistry & Materials

GOLD OPEN ACCESS

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

ROYAL SOCIETY OF CHEMISTRY

Industrial Chemistry & Materials

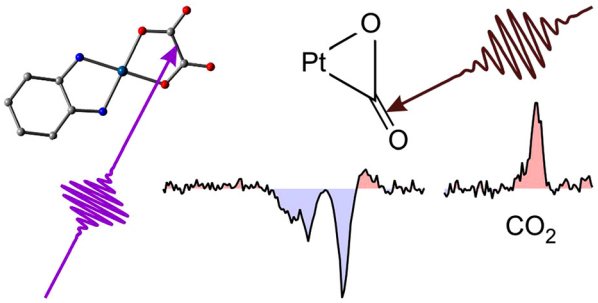
Open Access Article. Published on 06 March 2025. Downloaded on 2/1/2026 4:03:59 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

5012

Photoinduced formation of a platina-α-lactone – a carbon dioxide complex of platinum. Insights from femtosecond mid-infrared spectroscopy

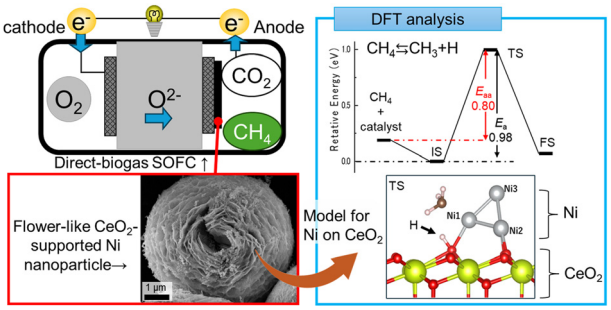
Markus Bauer, Raphaela Post, Luis I. Domenianni and Peter Vöhringer*



5024

Investigating Ni nanoparticles on CeO_2 for methane dissociation: a comparative study of theoretical calculations and experimental insights

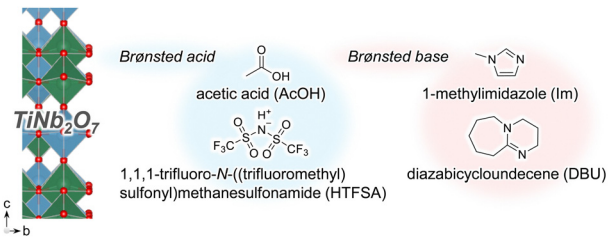
Takaya Fujisaki,* Yuta Tsuji, Phuc Hoan Tu, Tin Chanh Duc Doan, David S. Rivera Rocabado, Aleksandar Tsekov Staykov, Keiji Yashiro and Yusuke Shiratori*



5037

Electrochemical protonation/deprotonation of $TiNb_2O_7$ in protic ionic liquids

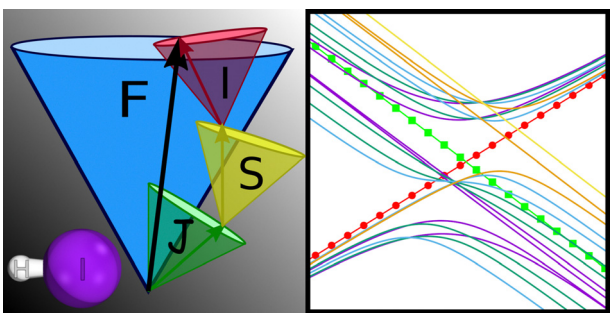
Masahiro Shimizu,* Takuya Kawai, Tomonori Ichikawa and Susumu Arai



5043

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

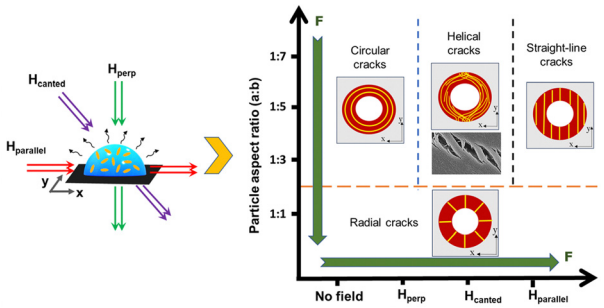
Maik Vossel, Iordanis Tsakontsis, Nicole Weike and Wolfgang Eisfeld*



Open Access Article. Published on 06 March 2025. Downloaded on 2/1/2026 4:03:59 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

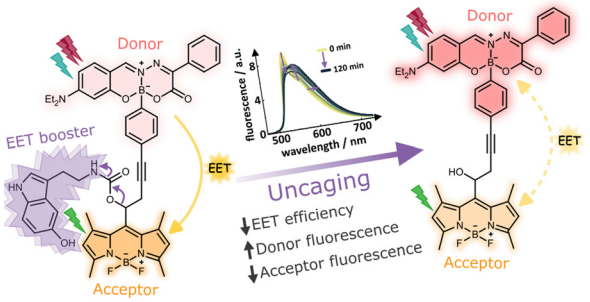
5056



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

Deeksha Rani* and Subhendu Sarkar

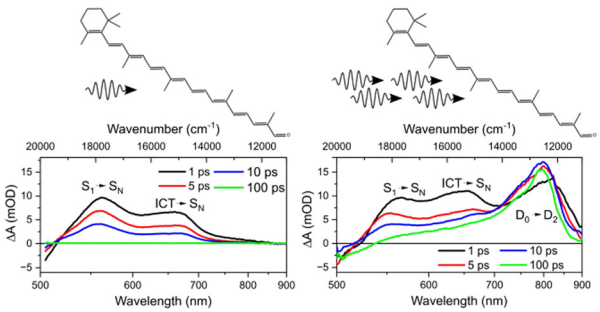
5064



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*

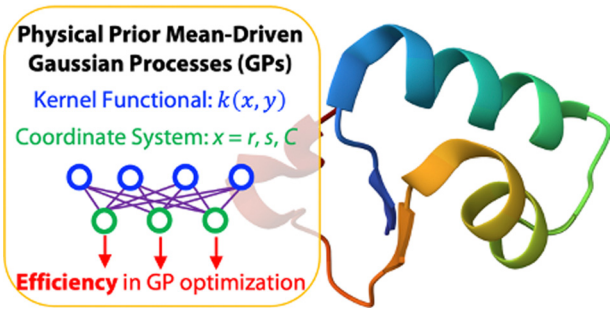
5080



Carotenoid radical formation after multi-photon excitation of 8′-apo-β-carotenal

Václav Šebelík, Valentyna Kuznetsova, Ivana Šímová 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*

This journal is © the Owner Societies 2025

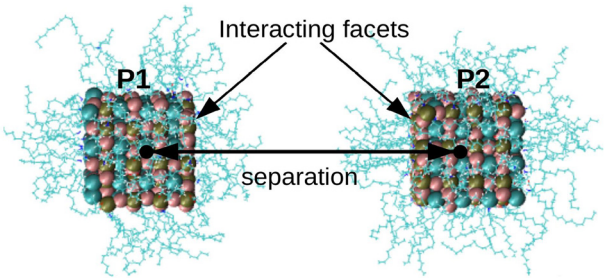
Open Access Article. Published on 06 March 2025. Downloaded on 2/1/2026 4:03:59 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

5098

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

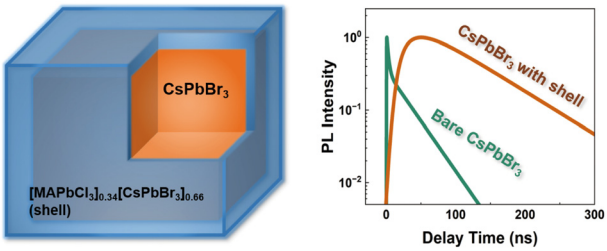
Avik Sasmal,* Edwine Tendong,* Tanusri Saha-Dasgupta and Jaydeb Chakrabarti



5109

Carrier recombination dynamics in $[MAPbCl_3]_x[CsPbBr_3]_{1-x}$ shell-passivated $CsPbBr_3$ single crystals

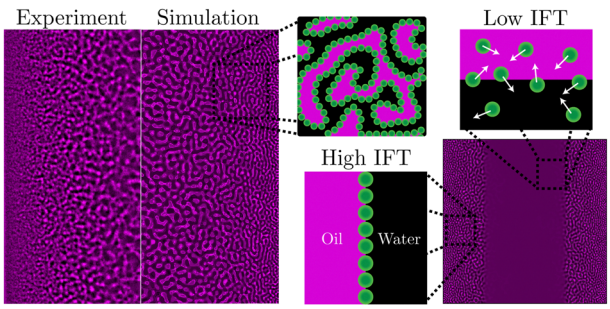
Zheng Zou, Zijie Xiao, Wenxin Dong, Wei Dang,* Shusheng Pan, Xiaojun Su and Wei Zhang*



5117

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

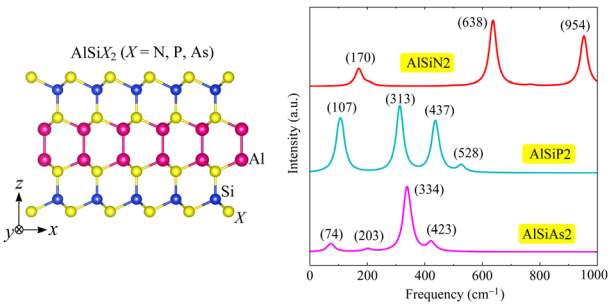
Jesse M. Steenhoff* and Martin F. Haase*



5131

Two-dimensional piezoelectric $AlSiX_2$ (X = N, P, As) semiconductors with Raman activity, favorable band-gap, and high carrier mobility based on first-principles calculations

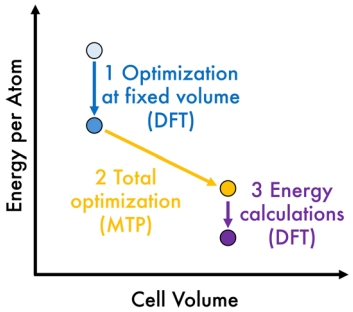
Tuan V. Vu, Nguyen N. Hieu, Nguyen T. Hiep, Thuat T. Trinh, A. I. Kartamyshev and Huynh V. Phuc*



Open Access Article. Published on 06 March 2025. Downloaded on 2/1/2026 4:03:59 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

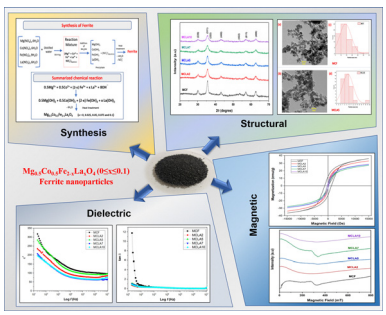
5141



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

Nikita Rybin,* Ivan S. Novikov and Alexander Shapeev

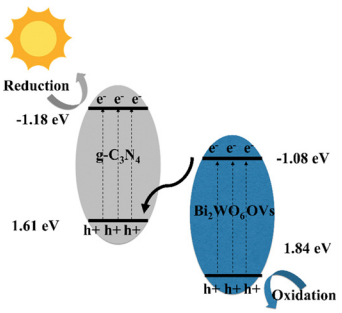
5149



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*

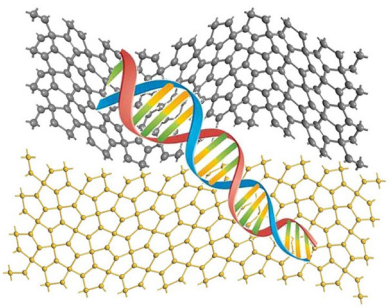
5163



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*

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*

This journal is © the Owner Societies 2025

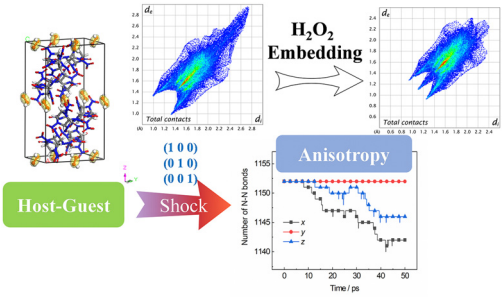
Open Access Article. Published on 06 March 2025. Downloaded on 2/1/2026 4:03:59 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

5186

Anisotropic initial reaction mechanism and sensitivity characterization of the host–guest structure CL-20/H_2O_2 under shock loading

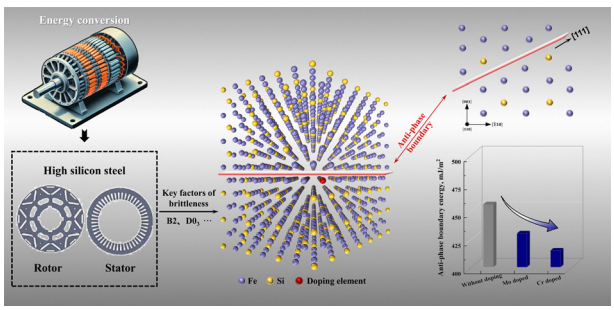
Yu Sha and Xiaobing Zhang*



5198

Effects of doping on anti-phase boundaries and the magnetic properties of the $D0_3$ structure in high silicon steel: first-principles insights

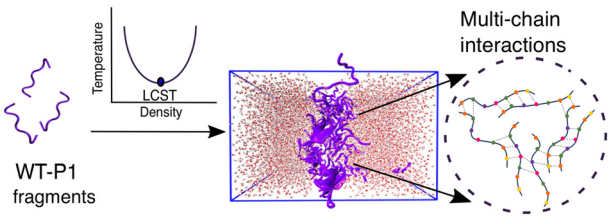
Meng Sun, Linxian Li, Hongyu Song, Shuai Tang,* Qing Peng,* Guichang Shen, Tianwei Xie, Fengliang Tan and Zhenyu Liu



5206

Insight into the thermo-responsive phase behavior of the P1 domain of α-synuclein using atomistic simulations

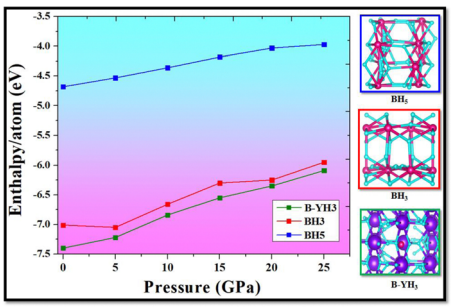
Sanchari Chakraborty and Mithun Biswas*



5215

Electron doping in non-magnetic YH_3 leads to room temperature ferromagnetism and a flat band: insights from density functional theory

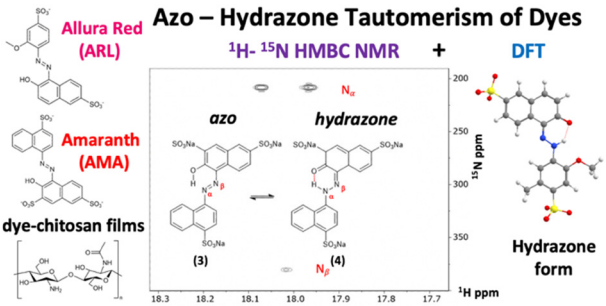
Pratap Mane, Ravi Kumar Trivedi, Parthasarathy Velusamy and Brahmananda Chakraborty*



Open Access Article. Published on 06 March 2025. Downloaded on 2/1/2026 4:03:59 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

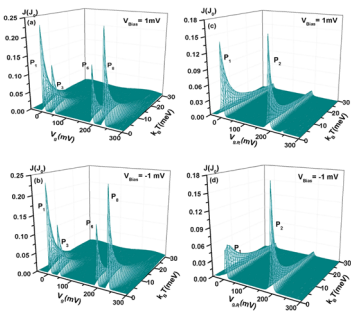
5228



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*

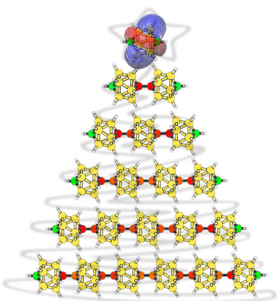
5238



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

David M. T. Kuo

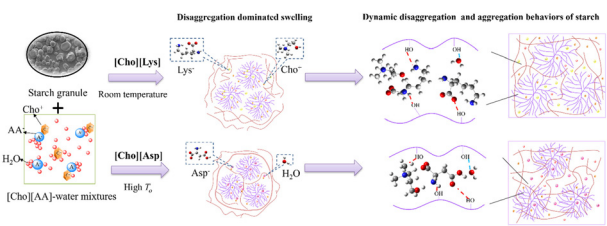
5249



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*

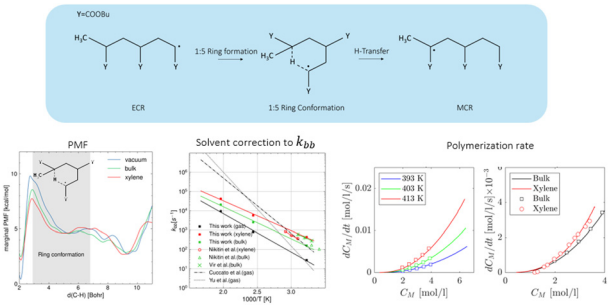
This journal is © the Owner Societies 2025

Open Access Article. Published on 06 March 2025. Downloaded on 2/1/2026 4:03:59 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

5271

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

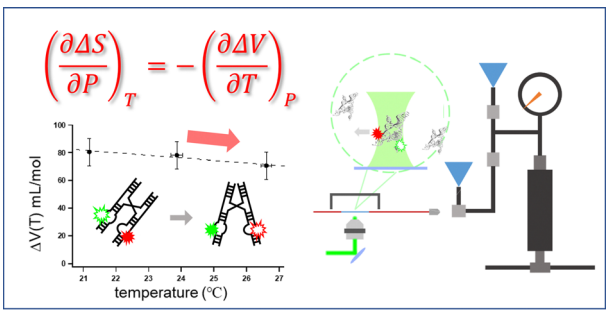
Francesco Serse,* Matteo Salvalaglio and Matteo Pelucchi*



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

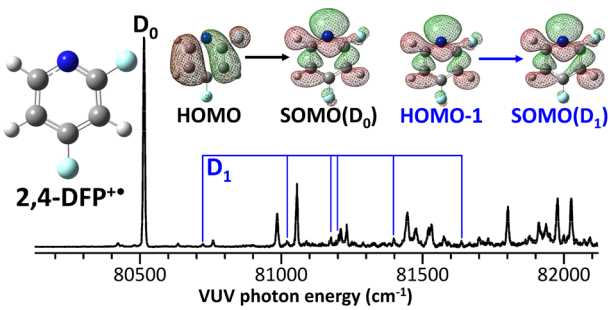
Hsuan-Lei Sung and David J. Nesbitt*



5296

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

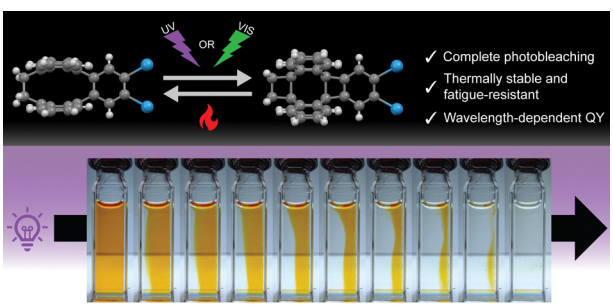
Hyojung Kim, Sung Man Park and Chan Ho Kwon*



5305

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

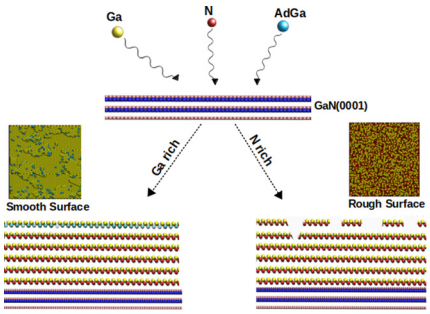
Kevin Lam, Robert J. Dillon, Abel Carreras,* Tomohiko Nishiuchi, Takashi Kubo,* Rabih O. Al-Kaysi, David Casanova and Christopher J. Bardeen*



Open Access Article. Published on 06 March 2025. Downloaded on 2/1/2026 4:03:59 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

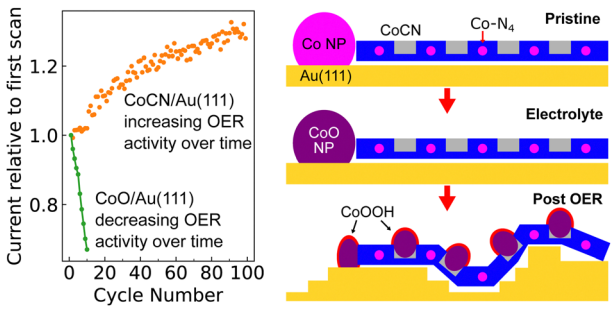
5317



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

Razia and Madhav Ranganathan*

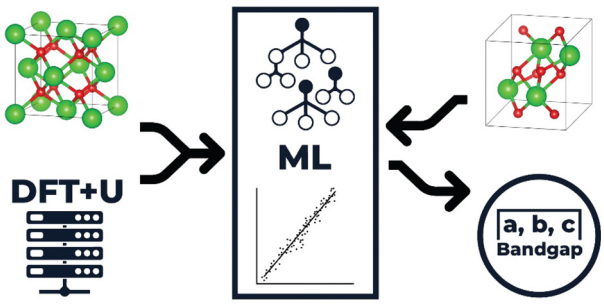
5326



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*

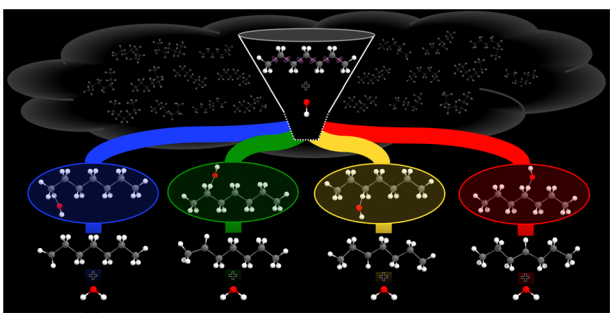
5338



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

This journal is © the Owner Societies 2025

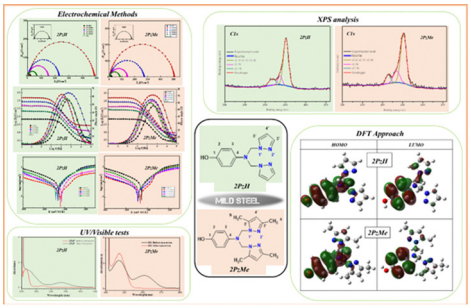
Open Access Article. Published on 06 March 2025. Downloaded on 2/1/2026 4:03:59 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

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

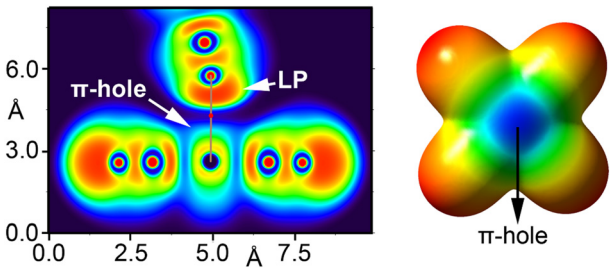
N. Setti, A. Barrahi, M. Maatallah, Y. Kaddouri, R. Touzani, B. Dikici, K. Karrouchi, Hatem A. Abuelizz, A. Zarrouk* and A. Dafali*



5395

Exploring coinage bonding interactions in $[Au(CN)_4]^-$ 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 X_2Y_3 (X = As, Sb, Bi; Y = Se, Te) using first-principles

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