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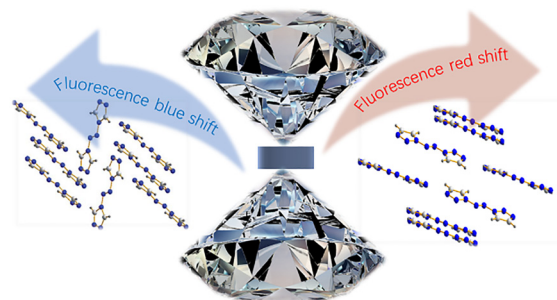
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pp. 7850–7856.
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COMMUNICATIONS

7826

Tunable piezochromic luminescence *via* isomer control in *N,N'*-azotriazole energetic molecules

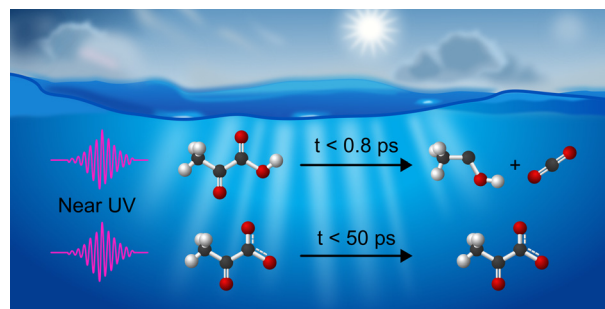
Meng-Zhou Guan, Yi-Lin Cao, Ying-Hui Liu, Li-Li Wang, Yu-Chuan Li* and Kai Wang



7830

The primary near-UV photochemistry of aqueous pyruvic acid

Jan Thøgersen, Tobias Weidner and Frank Jensen*



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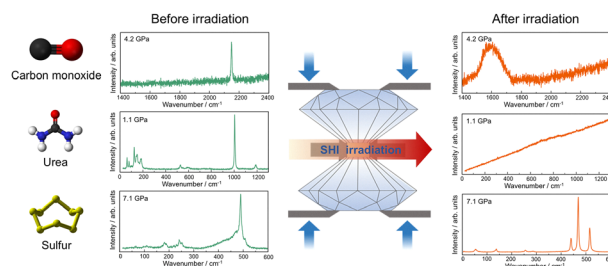
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Structural and optical responses of molecular solids to swift heavy ion irradiation under high pressures

Jiaxu Liang,* Lkhamsuren Bayarjargal, Ioannis Tzifas, Roman Belikov, Lena Wedek, Christopher Schröck, David Merges, Kay-Obbe Voss, Pascal Simon, Christina Trautmann, Maria Eugenia Toimil-Molares and Björn Winkler

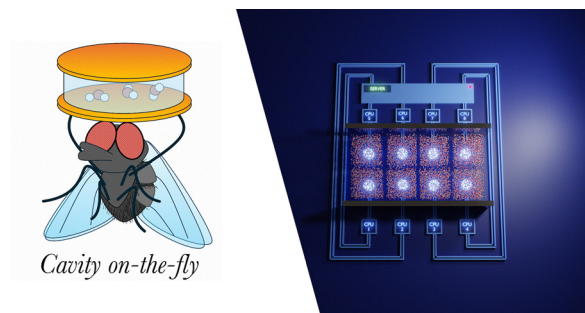


RESEARCH PAPERS

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On-the-fly cavity–molecular dynamics of vibrational polaritons

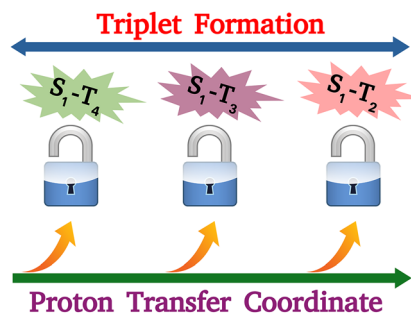
Sachith Wickramasinghe, Amirhosein Amini and Arkajit Mandal*



7850

Proton transfer-driven intersystem crossing in apigenin

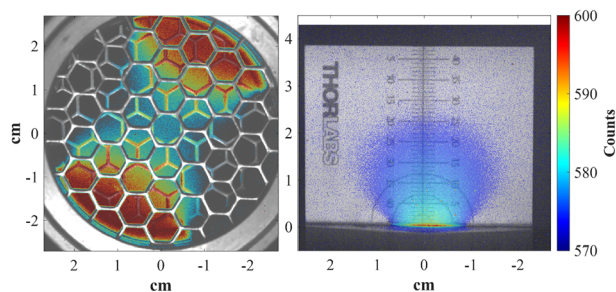
Sharan Babu, Anshuman Bera and Sivaranjana Reddy Vennapusa



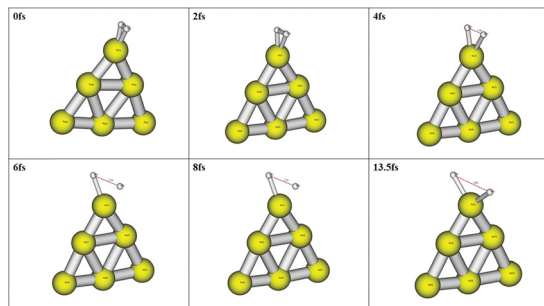
7857

Spectroscopic analysis of the $N_2 B^3\Pi_g - A^3\Sigma_u^+$ in radiation-induced air ionization

C. M. Murzyn, E. R. Jans and G. J. Marshall*



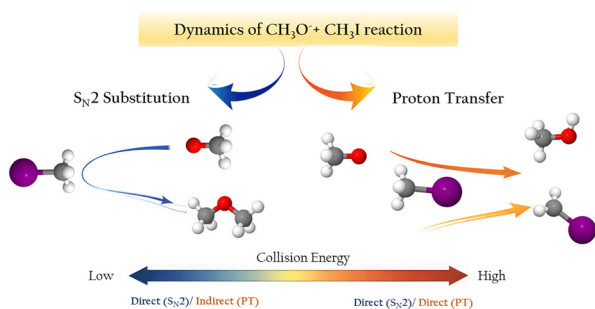
7869



Trajectory surface hopping study of photocatalyzed H₂ dissociation on a gold cluster

Prabhash Mahata and George C. Schatz*

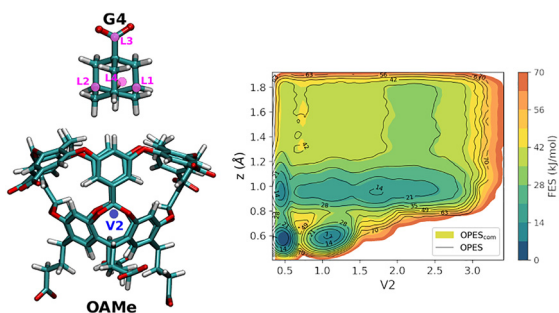
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Direct chemical dynamics simulations of the CH₃O⁻ + CH₃I reaction: substitution vs. proton transfer

Anitta Regina, Akash Gutal and Manikandan Paranjothy*

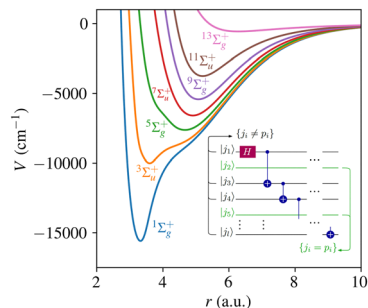
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Free energy landscapes of host-guest binding from adaptive bias enhanced sampling

Revanth Elangovan and Dhiman Ray*

7900



Advantages of discrete variable representation in variational quantum eigensolvers for vibrational energy calculations

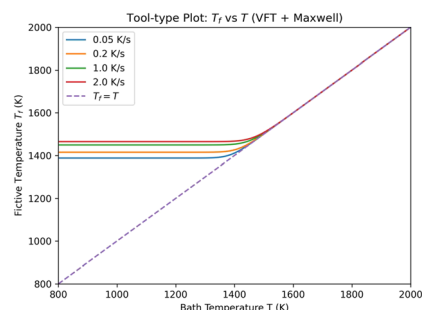
K. Asnaashari,* D. Bondarenko and R. V. Krems



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Fictive temperature of a glassy system in terms of frequency-dependent specific heat: a memory function approach

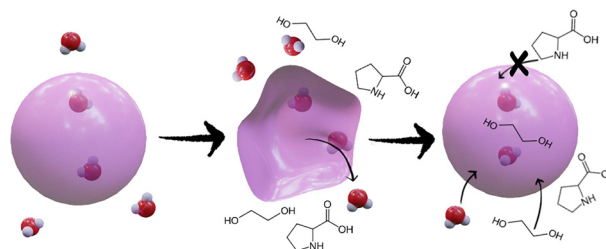
Biman Bagchi



7922

Insights into the molecular association of aqueous deep eutectic solvents using cell permeability

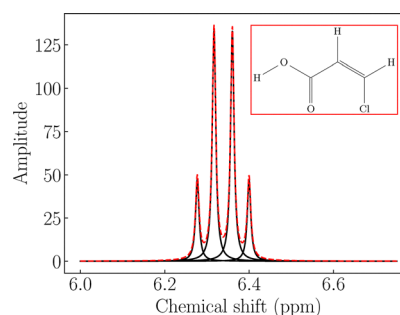
Saffron J. Bryant,* Miyah N. Awad, Amanda N. Abraham, Izabela Mitogrodzka, Tamar L. Greaves and Gary Bryant



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Study of nuclear magnetic resonance spectra with the multi-modal multi-level quantum complex exponential least squares algorithm

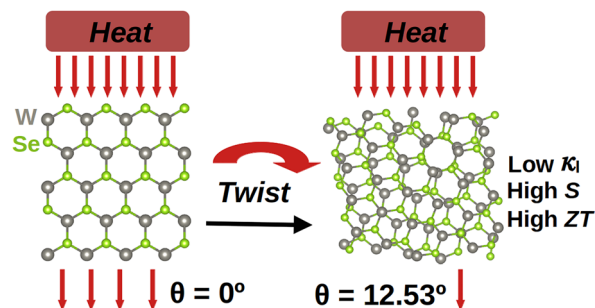
Antonio Márquez Romero, Josh J. M. Kirsopp, Giuseppe Buonaiuto and Michal Krompiec



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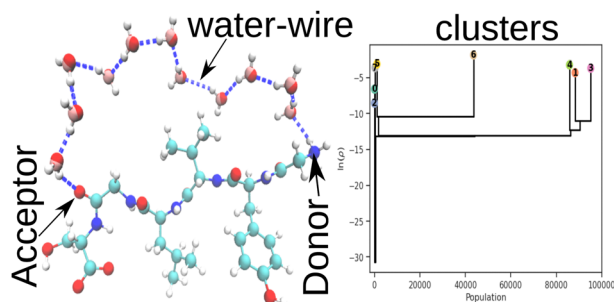
Moiré-pattern-assisted thermoelectric enhancement in tungsten diselenide bilayer

Naveen Kumar, Soumya Mondal and Ayan Datta*



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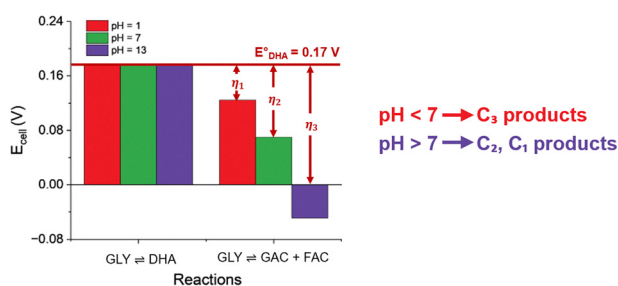
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Graph-based analysis of H-bond networks and unsupervised learning reveal conformational coupling in prion peptide segments

Wycliffe Omwansu,* Robinson Musembi and Solomon Derese

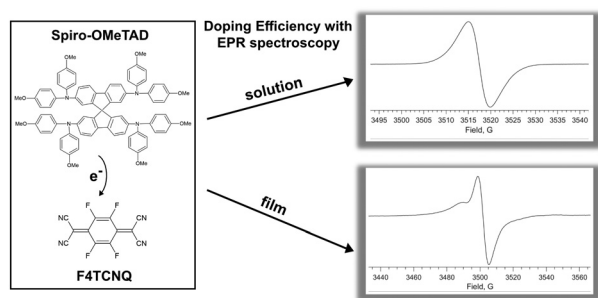
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Thermodynamics of the glycerol oxidation reaction: effect of temperature, pH, applied potential, and concentration

Andrés F. Pérez-Torres,* Roel van de Krol and Marco Favaro*

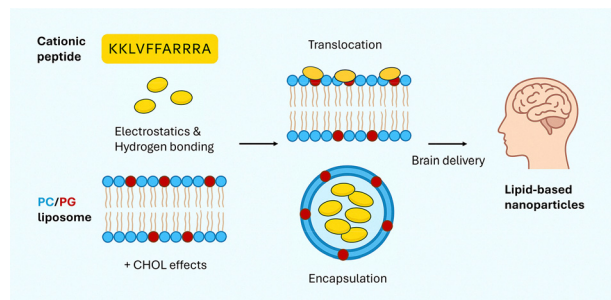
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Characterization of F4TCNQ as a dopant in spiro-OMeTAD thin films by electron paramagnetic resonance spectroscopy

Shipra Prakash,* Carl Hägglund, Shaoqi Zhan, Bhavya Rakheja, Gerrit Boschloo and Fikret Mamedov*

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Molecular dynamics insights into the interactions of a potential neurotherapeutic peptide with model liposomes

Gulsah Gul

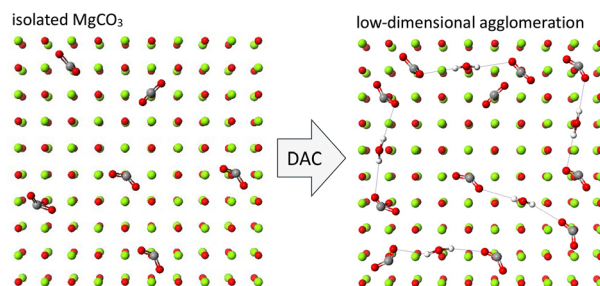


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8001

CO₂ direct air capture in the early hydration stage for light-burned MgO: a low-dimensional agglomeration regime

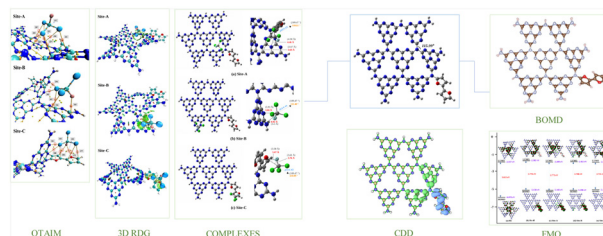
Eri Inoue and Kiminori Sato*



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DFT investigation of electronic modulation and site specific CFC-11 sensing on difuran functionalized heptazine based g-C₃N₄

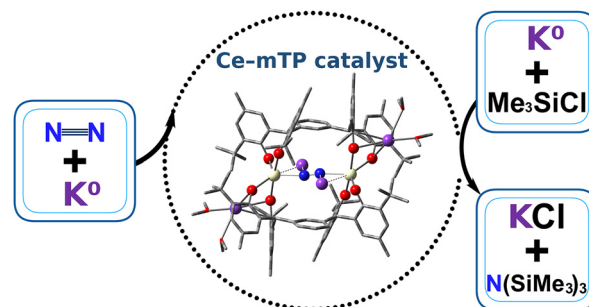
Hrishipad Deka and Dhruva Jyoti Kalita*



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Electron–electrophile coupled dinitrogen reduction in a cerium–*meta*-tetraphenolate system: a computational study

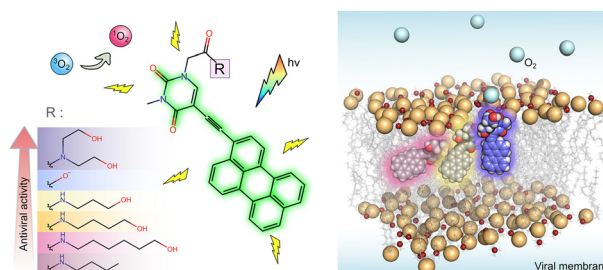
Shahbaz Ahmad, Polly L. Arnold* and Nikolas Kaltsoyannis*



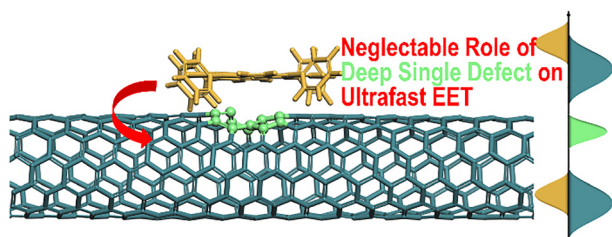
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Towards molecular dynamics simulation of membrane-targeting photosensitizing antivirals

Irina S. Panina, Yulia S. Vlasova, Yulia S. Panina, Maxim S. Krasilnikov, Vera A. Alferova, Vladimir A. Korshun and Anton O. Chugunov*



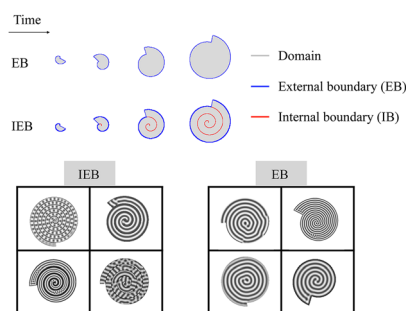
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The negligible effect of a single vacancy defect on ultrafast excitation energy transfer from porphyrin to single-walled carbon nanotubes

Xiao-Ying Xie, Ya-Qi Xu, Xi Zhao and Wen-Kai Chen*

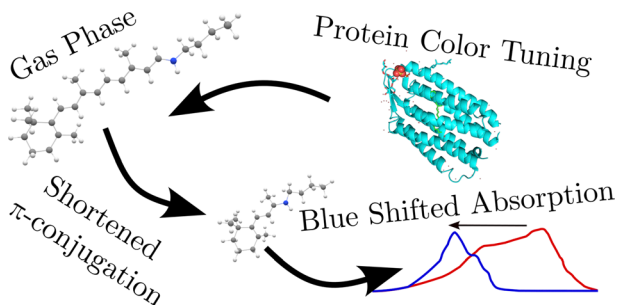
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Boundary effects on Turing pattern formation in a spiral growing domain

Leonardo Silva-Dias* and Milos Dolnik

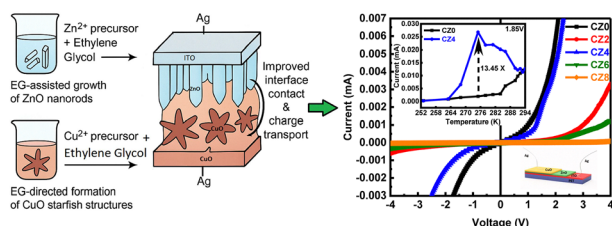
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Spectroscopy of cryogenic protonated Schiff-base retinal derivatives

Nikolaj Klinkby,* Anne P. Rasmussen, Anders G. S. Lauridsen, Mordechai Sheves and Lars H. Andersen

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Development of CuO–ZnO-based rectifying junctions for advanced electronic applications

Maruthi Mala,* Rajib Mahato and Anagh Bhaumik*

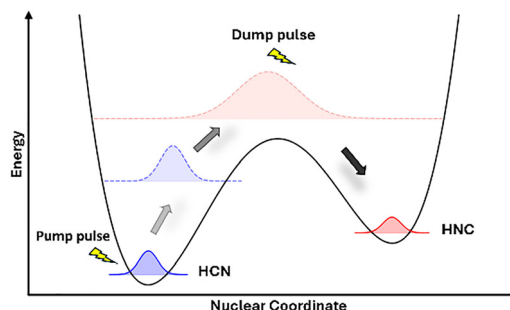


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Isomerization HCN → HNC in the electronic ground state using chirp-optimized mid-IR pump and dump laser pulses: 3D quantum dynamics

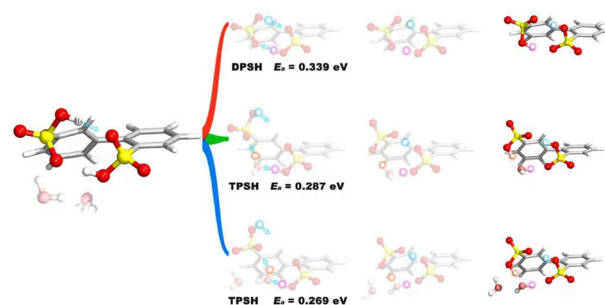
Kasper L. Effersø and Niels E. Henriksen*



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Theoretical elucidation of water-mediated multiple proton transport in sulfonates

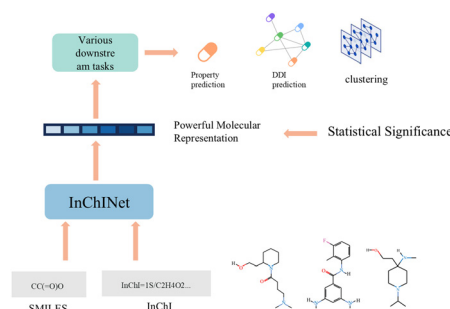
Longda Wei, Yitong Zhu, Jiasheng Wang, Weiwei Zeng, Chengkun Zhou, Yuqing Yan,* Bo Li* and Jingping Zhang*



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InChI-net: a self-supervised molecular representation learning framework leveraging SMILES and InChI

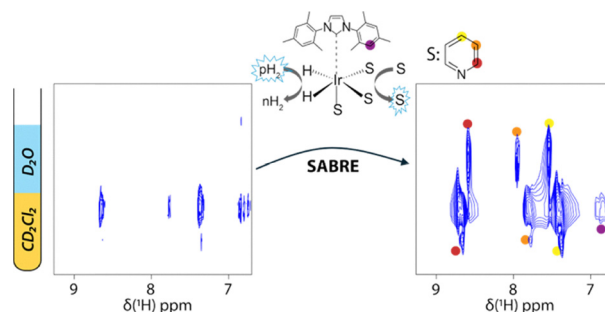
Yongna Yuan,* Jiahe Kang, Yuanchen Li, Ruisheng Zhang and Wei Su



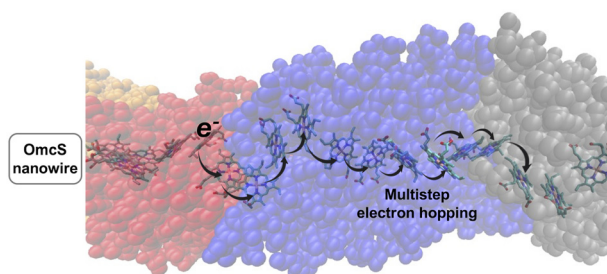
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NMR methods for characterizing molecular species in two immiscible solvents: application to SABRE-hyperpolarised species

Guillaume Verhaeghe, Gaspard Huber and Patrick Berthault*



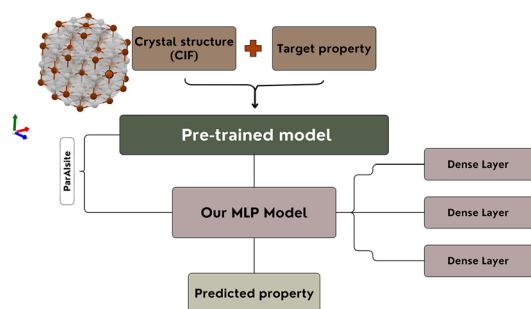
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Sources of non-Arrhenius electron transport in bacterial nanowires

Kiriko Terai, Peng Zhang and David N. Beratan*

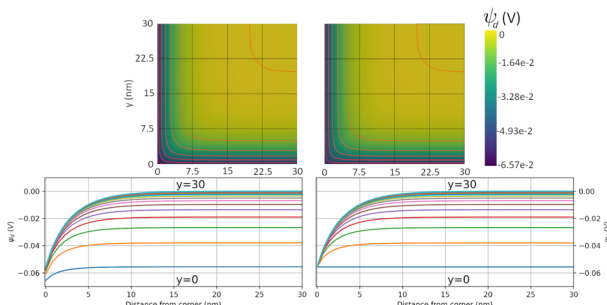
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Two-stage transfer learning for deep learning-based prediction of lattice thermal conductivity

Liudmyla Klochko* and Mathieu d'Aquin

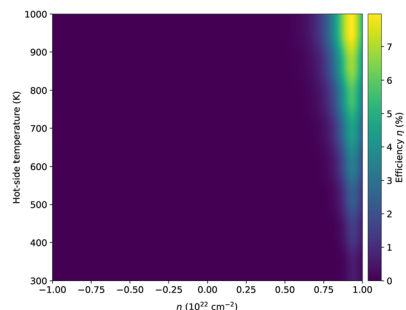
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Charge regulation and surface complexation modeling in nanoscale 2D geometries: benchmarking and test cases of a novel code (CRESCENDO)

Lasse Stausberg,* Frank Heberling and Johannes Lützenkirchen

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Thermoelectric properties of lead halide Janus layers - a theoretical investigation

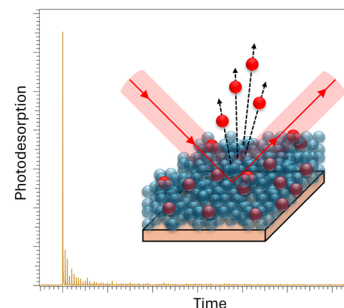
A. E. Sudheer, M. Vallinayagam,* G. Tejaswini, A. Kumar, M. Posselt, C. Kamal, M. Zschornak* and D. Murali*



8186

Infrared free electron laser induced photodesorption of CO and N₂ from solid amorphous water at cryogenic temperatures

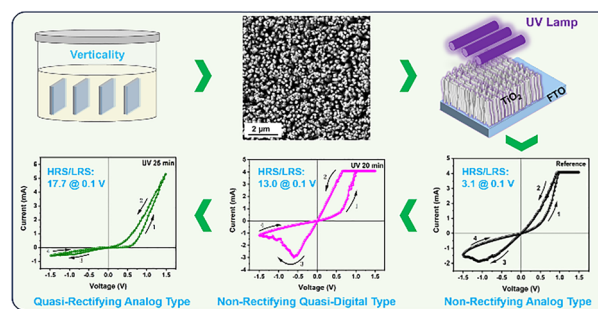
Kerry H. Jones, Jack E. Fulker,* Domantas Laurinavicius, Ali Ozel, Johanna. G. M. Schrauwen, Britta Redlich, Jennifer A. Noble, Sergio Ioppolo, Martin R. S. McCoustra and Wendy A. Brown*



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Controlled hydrothermal growth of uniform rutile TiO₂ nanorod arrays for memristive applications

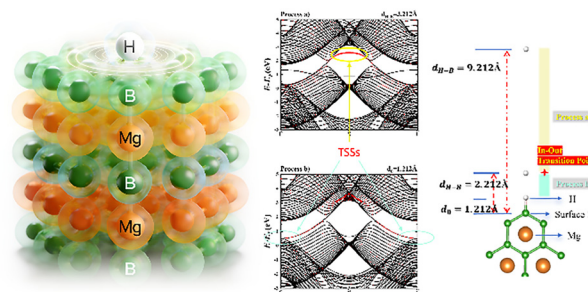
Zhiyuan Wang, Xiaohe Zhang, Yong Yang, Xiaobin Zhong, Suping Jia, Zongsheng Zhang, Yuan Gao, Junjie Guo* and Xiaoping Han*



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The study of hydrogen adsorption-induced topological surface state in-out hop in MgB₂ nodal-line semimetals via physics-informed Bayesian optimization

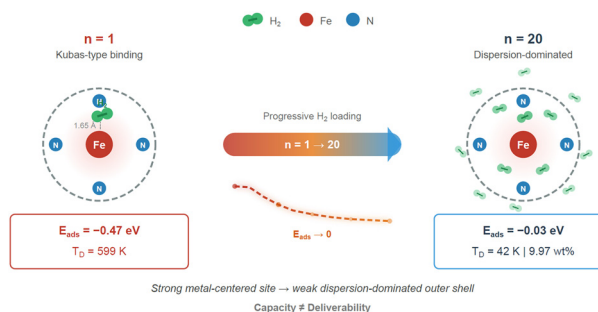
Qinchi Yue, Kun Bu,* Ruzhi Wang and Changhao Wang*



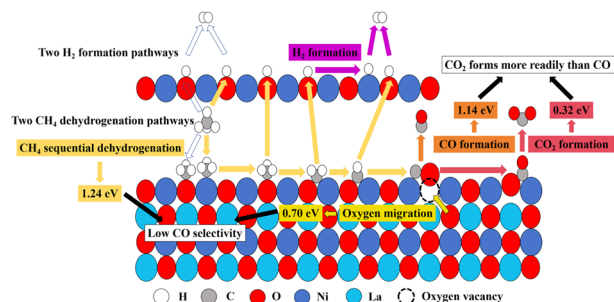
8225

Thermodynamics and electronic structure evolution from single-H₂ adsorption to stepwise hydrogen loading of Fe metalloporphyrin

Mustafa Kurban* and Iskender Muz



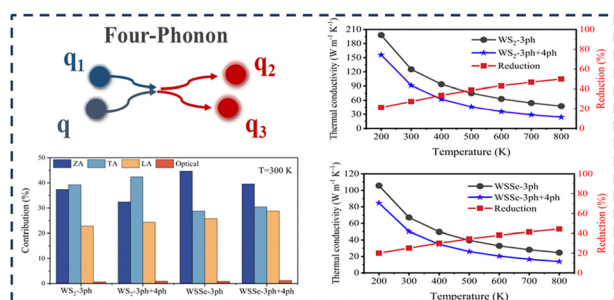
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Study of the methane reaction mechanism with a LaNiO₃ oxygen carrier in chemical looping reforming

Chenyao Wu, Hui Liu,* Yile Zou, Ruizhi Li, Jing Liu and Yanning Zhang*

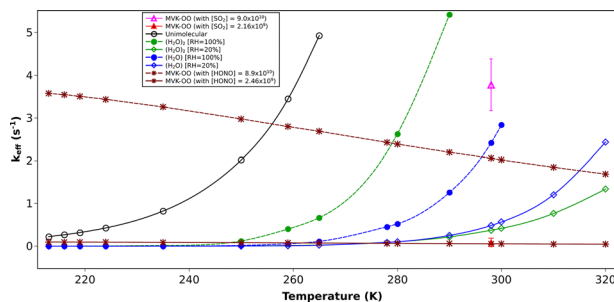
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The effect of four-phonon scattering on the lattice thermal conductivity of Janus WS₂ and WS₂ monolayers

Gang Liu,* Fengli Cao, Xiaodong Qiu and Weiwei Ju

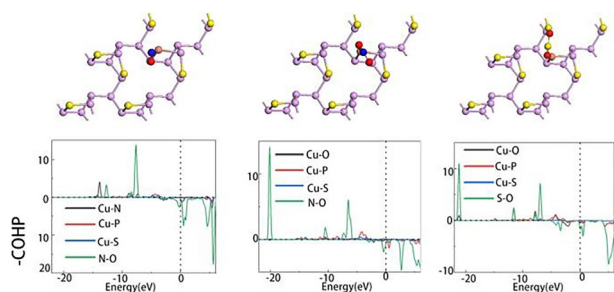
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HONO, a key sink of isoprene-derived Criegee intermediates (MACR-oxide and MVK-oxide)

Vishva Jeet Anand and Pradeep Kumar*

8277



Cu-doped P₃S-I monolayer: selective and robust toxic gas detection in ambient environments

Xuan Li, Li Shao,* Yuantao He, Yan Li and Jiehu Cui*



CORRECTIONS

8283

Correction: The influence of model building schemes and molecular dynamics sampling on QM-cluster models: the chorismate mutase case study

Donatus A. Agbaglo, Thomas J. Summers, Qianyi Cheng and Nathan J. DeYonker*

8285

Correction: Graph-based analysis of H-bond networks and unsupervised learning reveal conformational coupling in prion peptide segments

Wycliffe Omwansu,* Robinson Musembi and Solomon Derese

