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Cover

See Ricardo A. Mata, Paul Czodrowski, Stefan M. Kast *et al.*, pp. 18855–18869. Image reproduced by permission of Stefan M. Kast and Ricardo A. Mata from *Phys. Chem. Chem. Phys.*, 2025, 27, 18855.

EDITORIAL

18819

Introduction to Quantum bio-inorganic chemistry

Adam Kubas, Ragnar Bjornsson and Marcel Swart

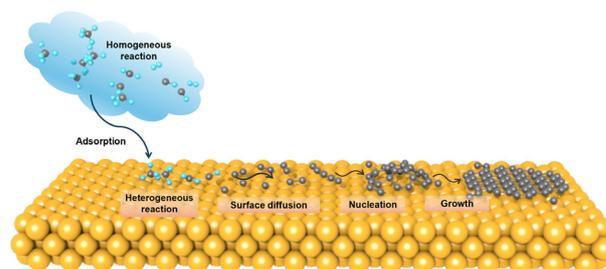


REVIEW

18821

Decoding complexity in chemical vapor deposition processes of two-dimensional materials via atomistic modeling

Zhengzheng Dang, Yide Chang, Jixin Wu, Zeyu Zhang, Zhichen Tang and Yanming Wang*



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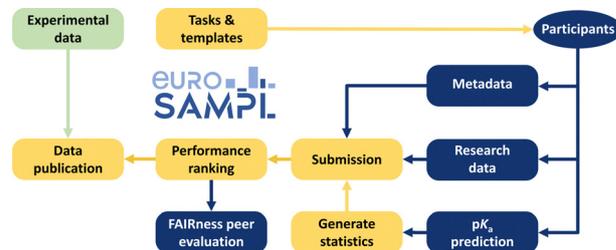


RESEARCH PAPERS

18855

The euroSAMPL1 pK_a blind prediction and reproducible research data management challenge

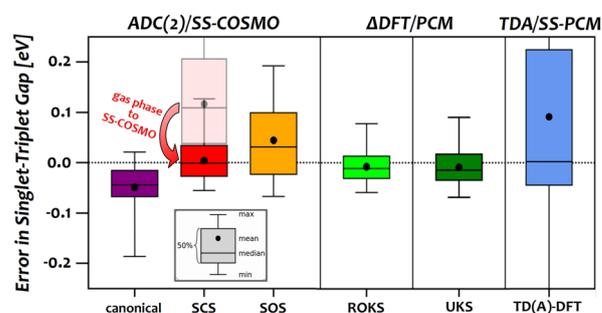
Nicolas Tielker, Michel Lim, Patrick Kibies, Juliana Gretz, Björn Hein-Janke, Christian Chodun, Ricardo A. Mata,* Paul Czodrowski* and Stefan M. Kast*



18870

Mind the gaps: what the STGABS27 set can teach about second-order excited state methods, solvent models, and charge transfer

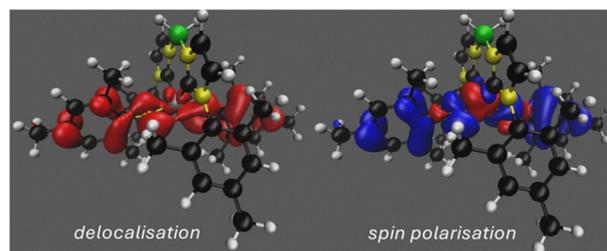
Thomas Froitzheim, Christof Hättig and Jan-Michael Mewes*



18887

First-principles paramagnetic NMR of a challenging Fe(v) bis(imido) complex: a case for novel density functionals beyond the zero-sum game

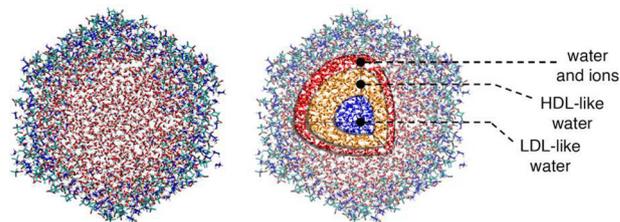
Ari Pyykkönen, Artur Wodyński, Martin Kaupp* and Juha Vaara*



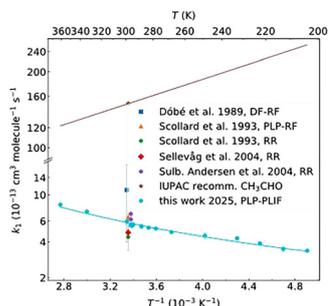
18901

Size-dependent effect of nano-confinement of water in an ionic liquid matrix at low temperature

Nico Di Fonte, Gianluca Dell'Orletta, Laura Zanetti-Polzi* and Isabella Daidone*



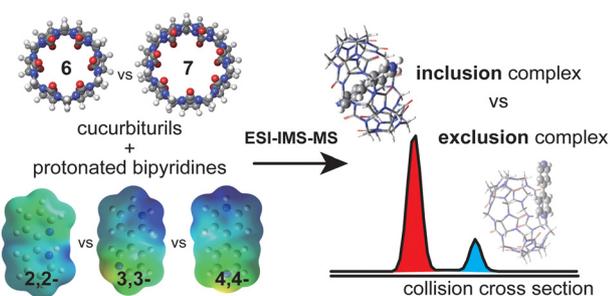
18907



Kinetics of the reaction of CF_3CHO with OH between 204 K and 361 K

Fabienne Baumann,* Christin Fernholz, Jos Lelieveld and John N. Crowley*

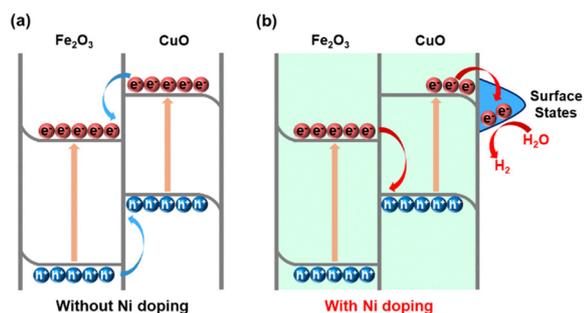
18917



Structures and energetics of protonated bipyridine–cucurbituril complex isomers in the gas phase

Doui Kim and Jongcheol Seo*

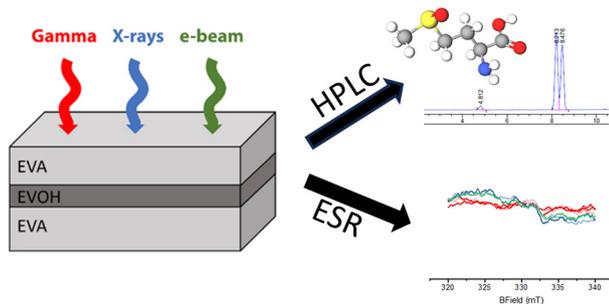
18927



Surface state activation driving charge separation via Z-scheme $\text{Fe}_2\text{O}_3/\text{CuO}$ heterojunctions for photocatalytic H_2 evolution

Ke Ma, Jingying Wei, Chun Gou, Huaiguo Xue, Jingqi Tian and Tengfei Jiang*

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Investigating dose rate effects and reactive species formation in irradiated multilayer films – part 1 EVA/EVOH/EVA

Blanche Krieguer,* Samuel Dorey,* Nathalie Dupuy,* Fabien Girard, Florent Kuntz, Nicolas Ludwig and Sylvain R. A. Marque*

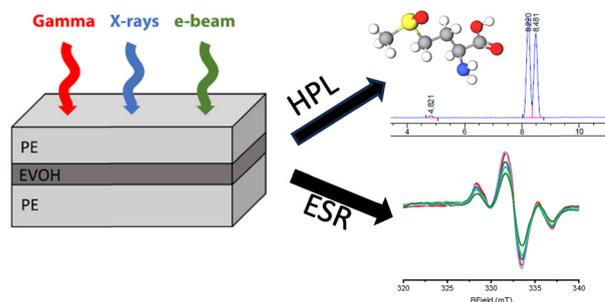


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18942

Investigating dose rate effects and reactive species formation in irradiated multilayer films – part 2 PE/EVOH/PE

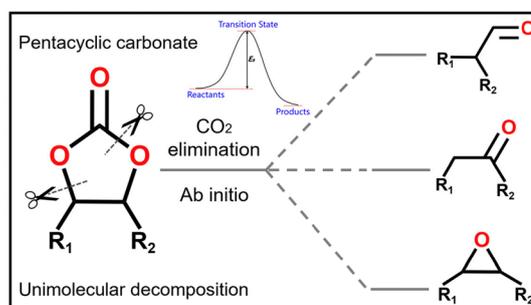
Blanche Krieguer,* Samuel Dorey,* Nicolas Ludwig, Florent Kuntz, Sylvain R. A. Marque,* Nathalie Dupuy* and Fabien Girard



18949

Unimolecular decomposition of pentacyclic carbonates: a computational kinetic study

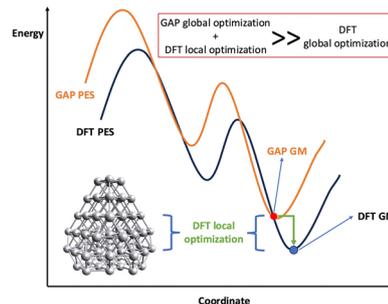
Zhi-Min Wang, Du Wang,* Wen-Jun Zhou, Ling-Nan Wu, Xu-Peng Yu and Zhen-Yu Tian*



18960

Parametrization of Gaussian approximation potential for the global optimization of magnesium clusters Mg_N ($N \leq 100$)

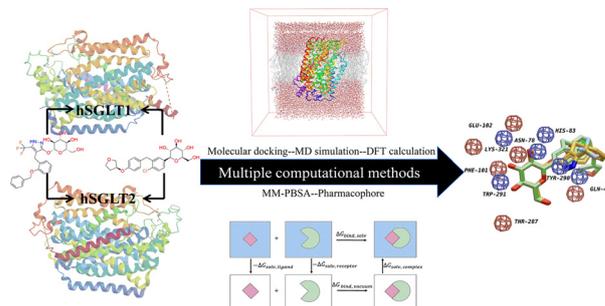
Ilya S. Steshin,* Sergey V. Pantelev, Igor V. Petukhov and Stanislav K. Ignatov



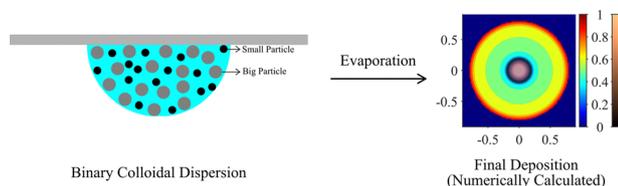
18978

Spatial and electronic features driving SGLT1/2 selectivity: a combined molecular dynamics and quantum mechanics study

Bingkun Chen, Baichun Hu, Yuxiang Zong, Yulong Wang, Lingyi Jing, Zihan Yu, Han Xue, Mingyang Hou and Xian Jia*



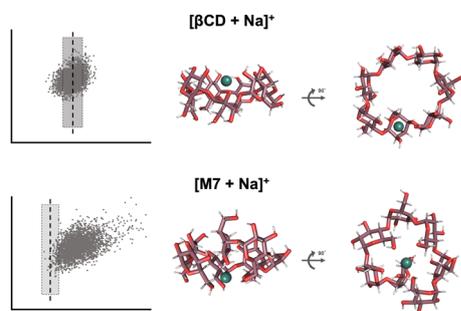
18997



Stratified patterns from evaporating colloidal dispersions containing binary particles

Logesh Kumar Pandurangan* and Janaki Vembu Murugesan

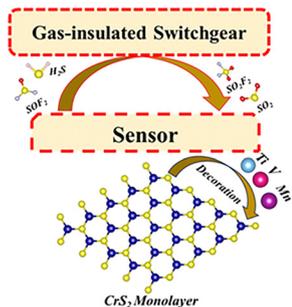
19006



Structural characterization of cyclodextrin and maltodextrin alkali-metal coordination *via* ion mobility-mass spectrometry and computational modeling

Hawkins S. Shepard, Emanuel Zlibut, Jody C. May, Benjamin K. Blakley and John A. McLean*

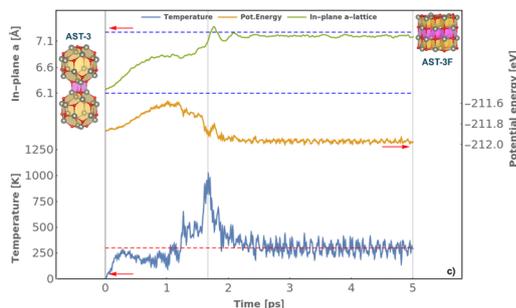
19016



A transition metal (Ti, V, and Mn)-decorated CrS₂ monolayer as a propitious gas scavenger for SF₆ decomposition remnants: acumen from density functional theory simulations

Sonam and Neetu Goel*

19030



Strain-driven phase transition in porous 2D AST-crystalline sheets: insights from DFTB+ simulations

Le Thi Hong Lien,* Thi Thao Nguyen and Vu Ngoc Tuoc

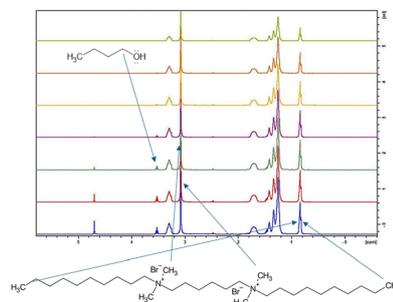


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Partition constants of alcohols and surfactants in mixed alcohol/10-carbon dimeric amphiphile aggregates from NMR-diffusion experiments

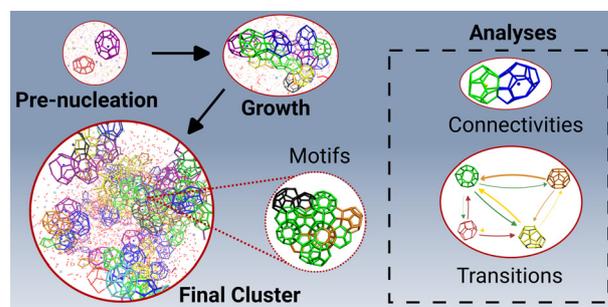
Ahmed A. Elgendy, Brooke A. Morris, Pratap Bahadur, Olivia M. Singer, Liah D. Christie, Robert D. Singer and D. Gerrard Marangoni*



19058

A study on a clathrate-like transition for carbon dioxide + propane + water via molecular dynamics simulations

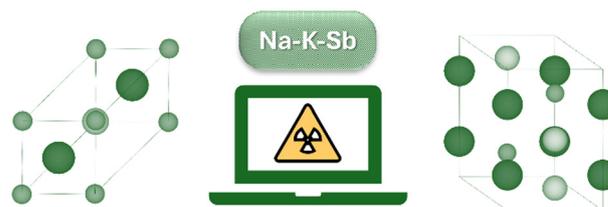
Arthur Benigno Weidmann, Luis Fernando Mercier Franco, Amadeu K. Sum and Pedro de Alcântara Pessoa Filho*



19071

Ab initio X-ray near-edge spectroscopy of sodium-based multi-alkali antimonides

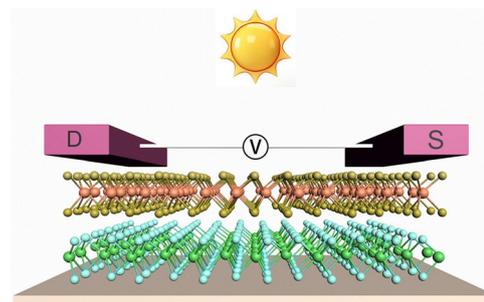
Chung Xu, Richard Schier and Caterina Cocchi*



19081

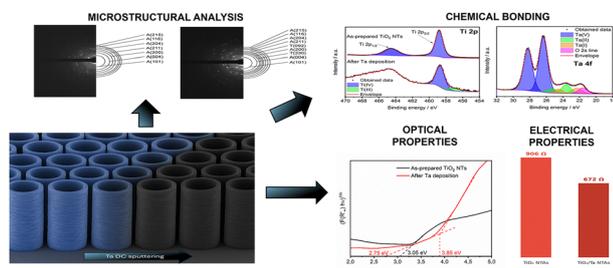
Strain-tunable MoSe₂/ZrCl₂ heterostructures: first-principles insights into photogalvanic and switching device performance

Zhonghui Xu, Hongyang Yu, Bing Luo,* Guogang Liu, Jiaxin Lu and Jie Kang



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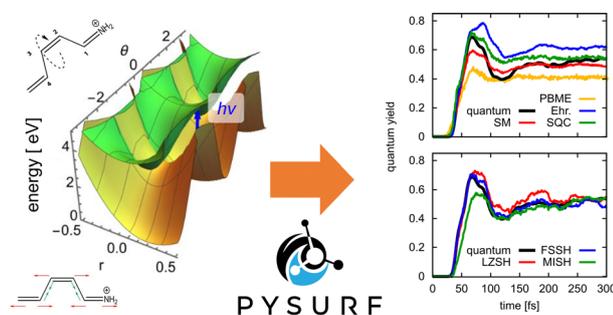
19092



Surface engineering of TiO₂ nanotubes with tantalum for improved electrochemical performance

Nemanja Latas, Dejan Pjević,* Jelena P. Georgijević, Dragana Jugović, Stevan Stojadinović and Nikola Cvjetičanin

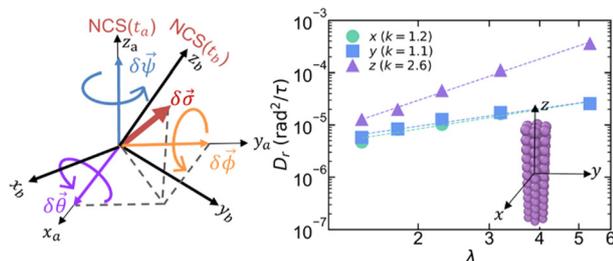
19105



Implementation of quasiclassical mapping approaches for nonadiabatic molecular dynamics in the PySURF package

David Picconi,* Maximilian F. S. J. Menger, Elisa Palacino-González, Edison X. Salazar and Shirin Faraji*

19123

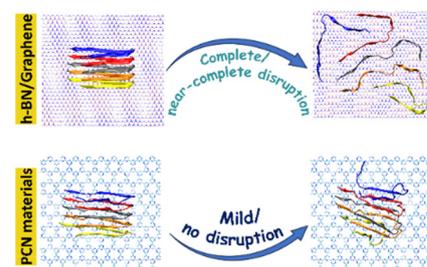


Decoupling three-dimensional rotational diffusion of anisotropic nanoparticles using small-angle approximation

Jia Zhang, Jiuling Wang, Hai-Xing Wang and Ruo-Yu Dong*

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Disruption of Aβ aggregate on nanomaterials



Two-dimensional materials can inhibit Aβ fibrillation in Alzheimer's disease

Anupam Ghosh, Titas Kumar Mukhopadhyay and Ayan Datta*

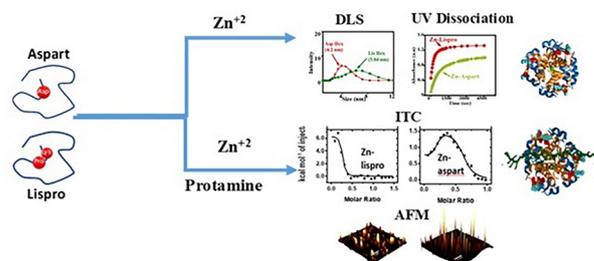


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Protamine and zinc binding-induced conformational effects on insulin analogs: an integrated experimental and computational study

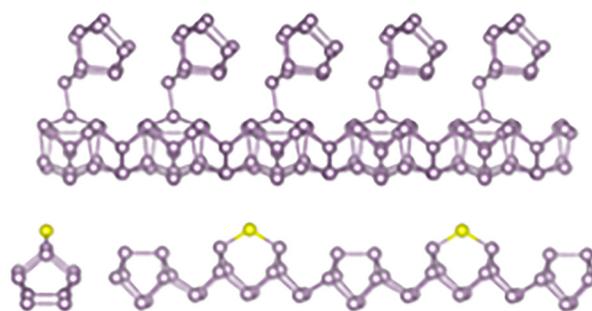
Pooja Dahiya, Priyanka Yadav, Ankit Singh, Soumya Aggarwal, Himanshu Joshi and Manoj Munde*



19163

Phosphorus nanotubes from chemical cleavage

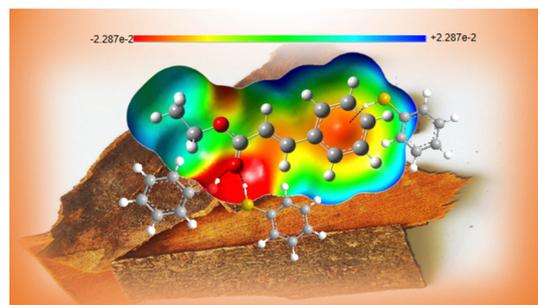
Romakanta Bhattarai and Xiao Shen*



19170

Modulations in the binding selectivity of phenol and thiophenol with ethyl cinnamate: an IR spectroscopic and quantum chemical investigation

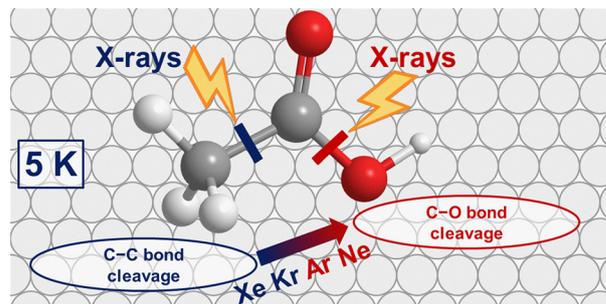
Puja Samanta and Pujarini Banerjee*



19181

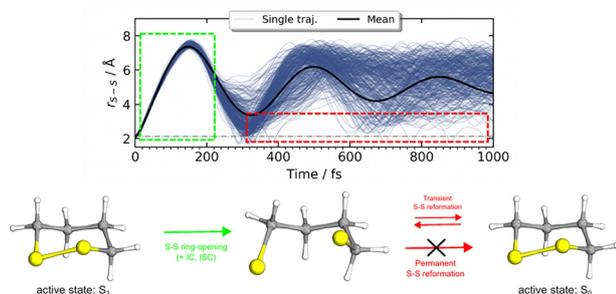
Radiation-induced degradation of acetic acid molecules in cryogenic media: diverse chemistry revealed by a matrix isolation FTIR study

Pavel V. Zasimov, Daniil A. Tyurin, Georgii A. Mirskoi, Elizaveta V. Sanochkina and Vladimir I. Feldman*



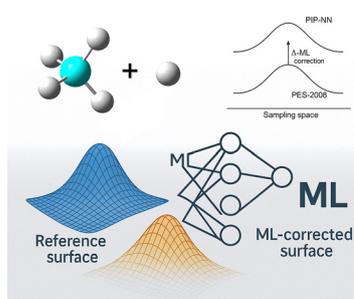
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**Triplets in the cradle: ultrafast dynamics in a cyclic disulfide**

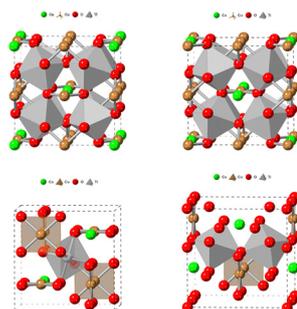
James Merrick, Lewis Hutton, Joseph C. Cooper, Claire Vallance* and Adam Kirrander*

19204

**Potential energy surfaces: Δ -machine learning from analytical functional forms**

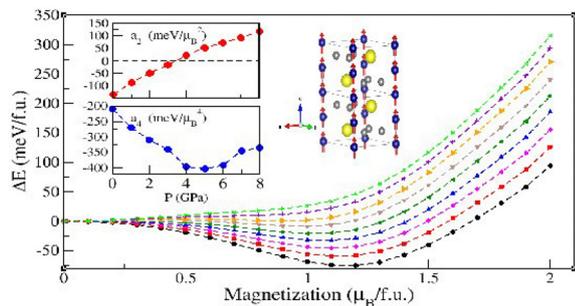
Cipriano Rangel* and Joaquin Espinosa-Garcia

19216

**Intrinsic polarization mechanism of CCTO based on optimized Skanavi model with displacement fields modification**

Xinrui Qin, Pengfei Cheng,* Hao Luo, Kejia Geng, Cuncun Kong, Xin Liu, Xueyan Su, Yaoheng Su and Dingze Lu

19224

**First-principles study of pressure effects on the physical, chemical and magnetic properties of LaCrGe₃**

Himanshu and J. J. Pulikkotil*

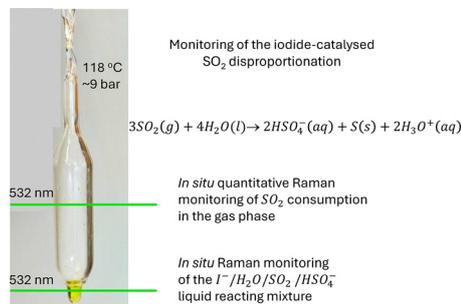


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SO₂ disproportionation for a sulphur-based thermochemical cycle studied in an *operando* Raman batch reactor

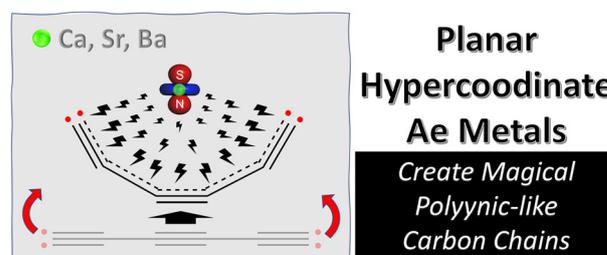
Theocharis Kentri, Loukas Kollias and Soghomon Boghosian*



19244

Planar tetra-, hexa-, octa-, and deca-coordinate Heavier alkaline-earth metals: covalent interactions of d orbitals with carbon chains

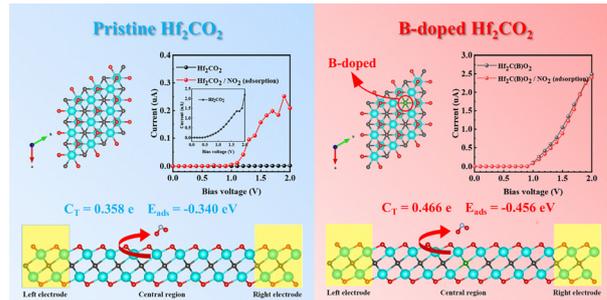
Xin-bo Liu, Yi-fan Yang, Li-juan Cui, Yu-le Dou and Zhong-hua Cui*



19254

Superior NO₂ sensing *via* semiconductor–metal transition in undoped Hf₂CO₂ MXene: doping-mediated trade-offs between surface reactivity and electronic properties

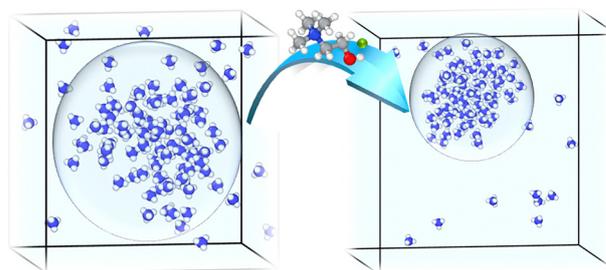
Renjie Zhu, Zebang Cheng, Wenjing Hu, Jiajun Jiang, Tingting Shi, Jing Chen, Xiaolin Liu, Lin Peng* and Jia Lin*



19265

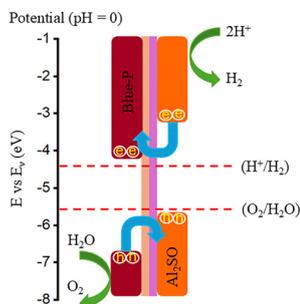
Unveiling the effect of choline chloride on hydrophobic association of methane

Pooja Nanavare and Rajarshi Chakrabarti*



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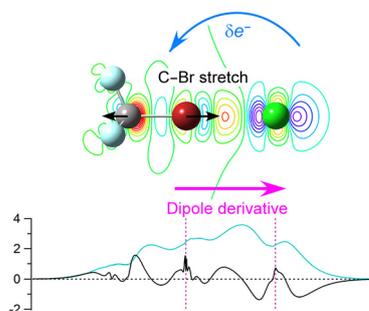
19283



First-principles prediction of SiS-Al₂SO and blueP-Al₂SO vdW heterostructures for high-efficiency photocatalytic water splitting with 23.67% solar-to-hydrogen conversion

Abid Raza, Ismail Shahid,* M. Munawar, Xiaoliang Zhang* and Dawei Tang

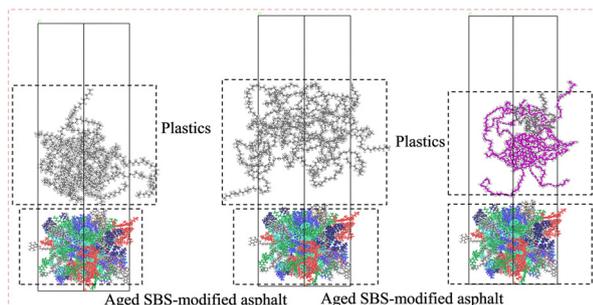
19295



Relative importance of electrostatic and intermolecular charge-transfer interactions in halogen bonding depending on the properties analyzed

Kyosuke Ino and Hajime Torii*

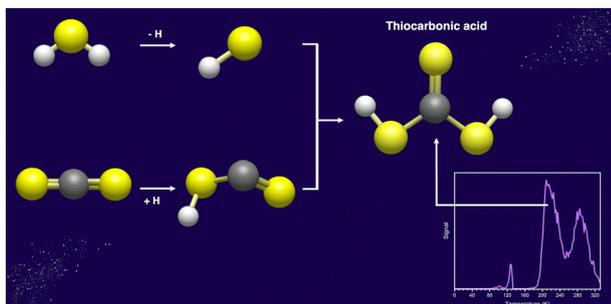
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Reutilization of waste polymer plastics: a molecular dynamics study on toughness enhancement and interfacial mechanisms in SBS-modified asphalt

Tengfei Nian,* Haowen Sun, Xinhui Li, Mingjuan Zhang, Wei Li and Piyi Li

19324



Formation of thiocarbonic acid (H₂CS₃) – the sulfur counterpart of carbonic acid (H₂CO₃) – in interstellar analog ices

Lina Coulaud, Jia Wang, Ashanie Herath, Andrew M. Turner, Mason Mcanally, Ryan C. Fortenberry* and Ralf I. Kaiser*

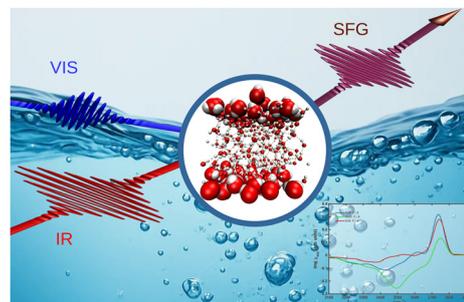


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Time-resolved vSFG of the water–air interface in an external field

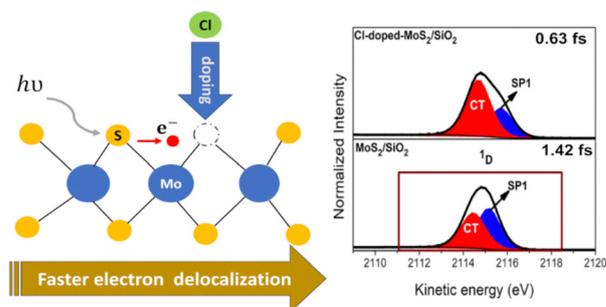
Deepak Ojha* and Thomas D. Kühne



19347

Anisotropic electron delocalization dynamics induced by chlorine doping in CVD-grown MoS₂ monolayers

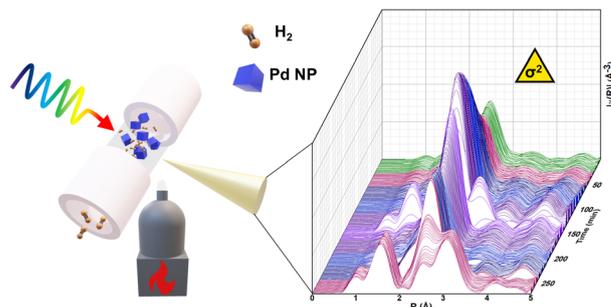
Yunier Garcia-Basabe,* Cesar D. Mendoza, Flávio C. Vicentin and Dunieskys G. Larrude



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Unraveling hydride dynamics on cubic palladium nanoparticles

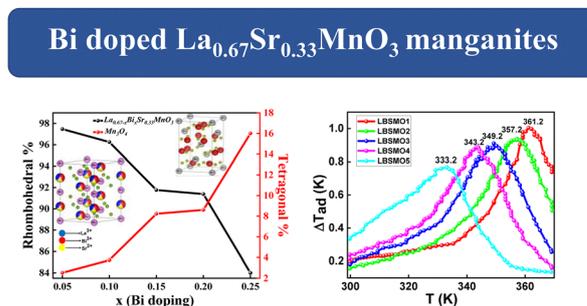
Marlon M. Silva, Esther M. Cunha, Valérie Briois and Amélie Rochet*



19365

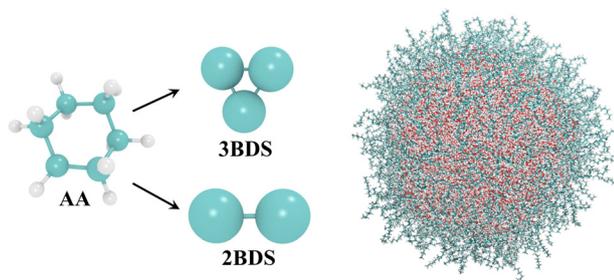
Tailored magnetic transitions and magnetocaloric properties towards room temperature in La_{0.67-x}Bi_xSr_{0.33}MnO₃ (x = 0.05–0.25) manganites

Parvathy Namboothiri, K. K. Supin, B. Arun, M. S. Anikin and M. Vasundhara*



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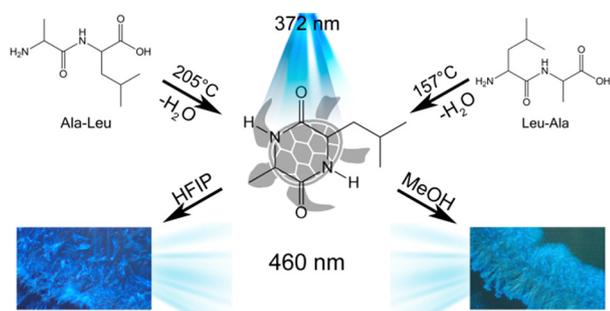
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Molecular dynamics of space-confined water inside Span 80 reverse micelles with an all-atom and coarse-grained solvent

Andrea Piserchia, Sergio Rampino,* Mirco Zerbetto, Francesca Tajoli, Silvia Gross and Antonino Polimeno

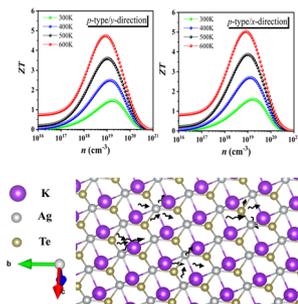
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Solid-state cyclization of Ala–Leu and Leu–Ala dipeptides, and self-assembly and luminescent properties of the cyclic dipeptide

Elina R. Mirgazieva, Radik A. Larionov, Sufia A. Ziganshina, Khasan R. Khayarov, Aleksandr E. Klimovitskii, Daria V. Tkachenko, Vladimir A. Burilov, Olga B. Babaeva, Artemiy G. Shmelev, Valery V. Gorbachuk and Marat A. Ziganshin*

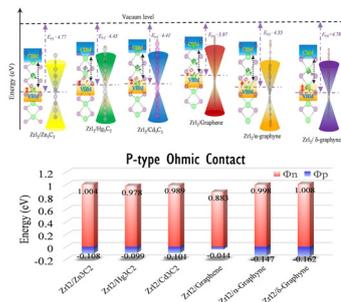
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Ultralow lattice thermal conductivity and enhanced thermoelectric performance in the AgKTe monolayer induced by four-phonon scattering

Qiong Meng, Chuan-Lu Yang,* Xiaohu Li, Yuliang Liu, Wenkai Zhao and Feng Gao

19410



Robust p-type ohmic contact in ZrI₂/Dirac semi-metal van der Waals heterostructures

Wu Zhang, Bo Li, Zhen-kun Tang and Liemao Cao*

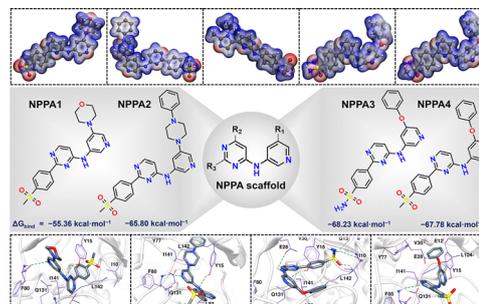


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***N*-(Pyridin-3-yl)pyrimidin-4-amine analogues as potent CDK2 inhibitors: an *in silico* investigative approach**

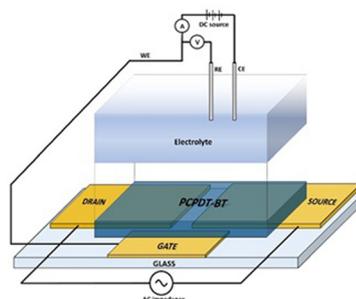
Muhammad Shafiq, Maria Nasim, Dmitry Nerukh, Mohammad Nur-e-Alam and Zaheer Ul-Haq*



19435

An unconventional electrochemical/solid-state-device integrated system: an electrochemical sensor based on the PCPDTBT polaronic state

Andrea Stefani, Camilla Ferrari, Agnese Giacomino, Sara Morandi, Andrea Marchetti, Suryakant Mishra and Claudio Fontanesi*



19445

Temperature dependence of reactions between aqueous manganese ions and water radiolysis products

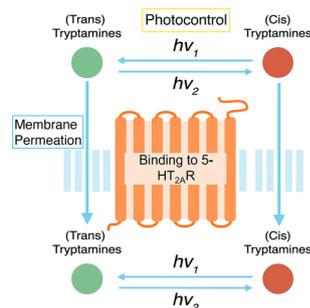
Aliaksandra Lisouskaya,* Ian Talty, Brady Soenen and Nevis Dickson



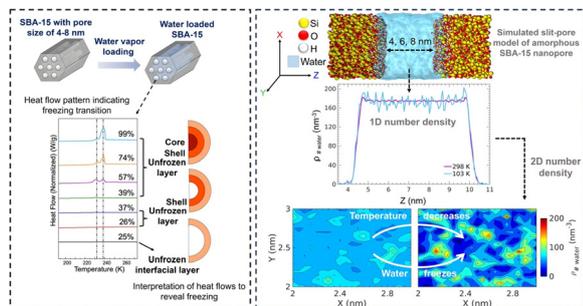
19454

Computational design of an improved photoswitchable psychedelic based on light absorption, membrane permeation and protein binding

Vito F. Palmisano, Claudio Agnorelli, Shirin Faraji* and Juan J. Nogueira*



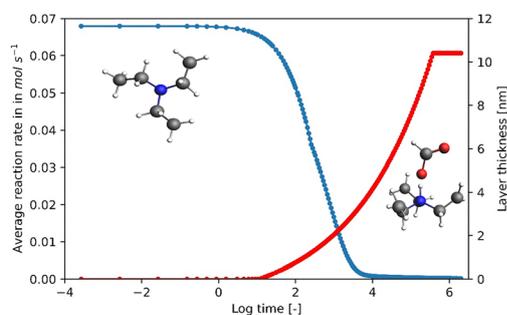
19465



Mechanisms underlying the freezing and melting behavior of water confined in silica nanopores as a function of pore size and pore filling

Yang Jia, Rituparna Hazra, Amy Wu, Sahil Mebul Patel and Greeshma Gadikota*

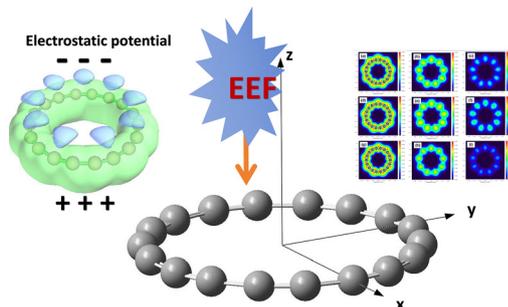
19480



Modelling of formic acid production using solventless trialkylamine reduction strategies

A. W. N. de Leeuw den Bouter, A. Miquelot, L. Brito, P. Olivier and J. van der Schaaf*

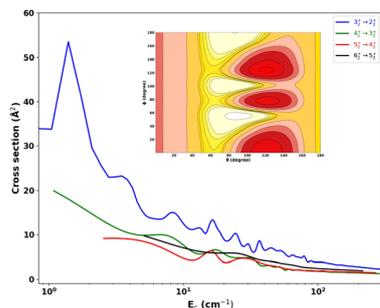
19488



How does an external electric field in the normal-direction affect the cyclo[18]carbon molecule?—a DFT study

Chuan Wang,* Blaž Likozar, Matej Huš,* Jie Wu, Ziqiu Wang and Kun Yang

19500



Rigid rotor state-to-state cross-sections and rates of the PH₃ + H₂ collision

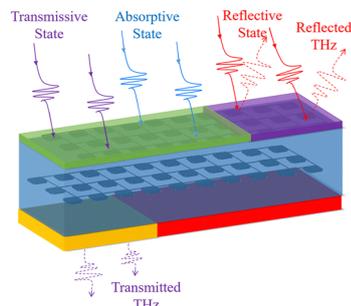
Faouzi Najar, Ayda Badri,* Hervé Tajou Tela, Steve Ndengué and Nicola Tassinato



19509

Design of multifunctional metasurface devices with tunable propagation properties

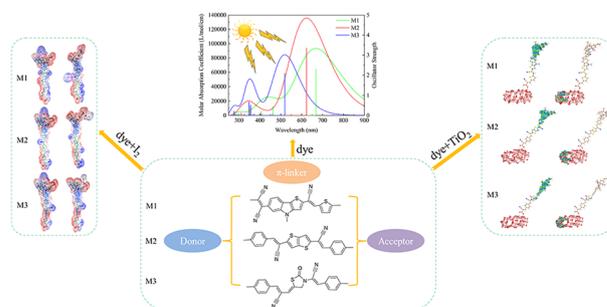
Usama Arif, Wei Su,* Jiang Yue, Muhammad Mohsin, Ahmad, Muhammad Fasih and Amna Inayat



19520

Insights into the sensitization effect and microscopic essence of π -linker structure regulation of metal-free organic dyes on the photovoltaic performance of dye-sensitized solar cells

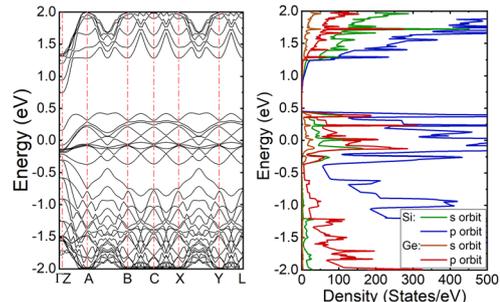
Meng-Dan Chen, Yan-Ren Lu, Xiao-Meng Zhao, Jie-Sheng Hu, Xiao Zhang and Xiao-Lin Wang*



19537

Impact of surface point defects on the electronic and optical properties of GeSi bulk materials

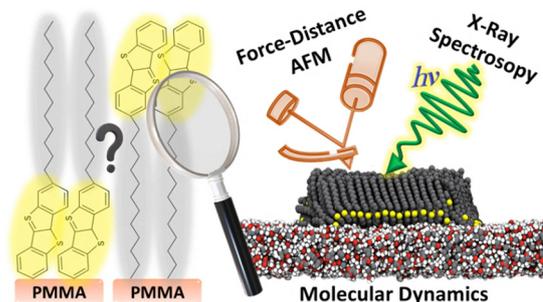
Hai Wan,* Haijuan Zhang, Huifeng Bi, Li Liu, Wanyu Zhao, Shuqi Wang and Qihang Lu



19546

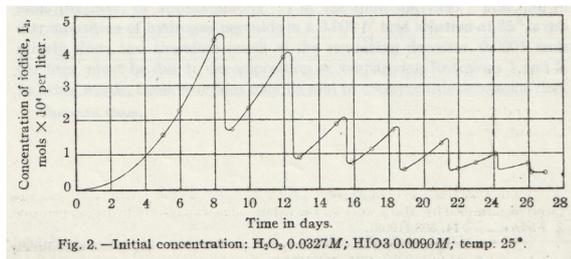
Molecular interplay at the PMMA dielectric and C₁₃-BTBT semiconductor interface

Kirill Gubanov, Dustin Vivod, Christiane Sauer, Maria Brzhezinskaya, Dirk Zahn and Rainer H. Fink*



COMMENTS

19553

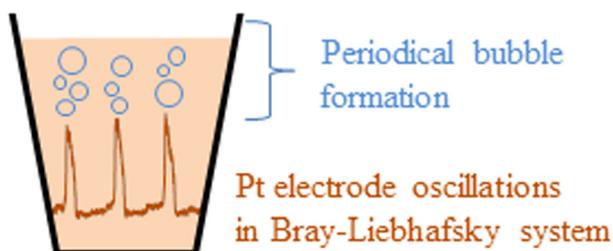
W. C. Bray, *J. Am. Chem. Soc.* 1921, 43, 1262

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Comment on “Experimental support for the model of Bray–Liebhafsky oscillatory reaction based on the heterogeneous effects” by I. N. Bujanja, A. F. Taylor and D. Stanisavljev, *Phys. Chem. Chem. Phys.*, 2024, 26, 24975

Guy Schmitz

19561



Reply to the ‘Comment on “Experimental support for the model of Bray–Liebhafsky oscillatory reaction based on the heterogeneous effects”’ by G. Schmitz, *Phys. Chem. Chem. Phys.*, 2025, DOI: 10.1039/D5CP00355E

Itana Nuša Bujanja, Annette Fiona Taylor and Dragomir Stanisavljev*

