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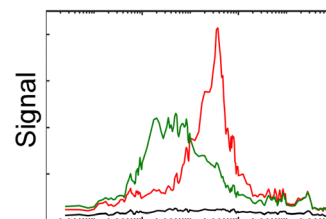
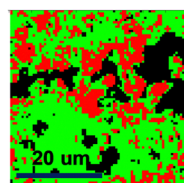
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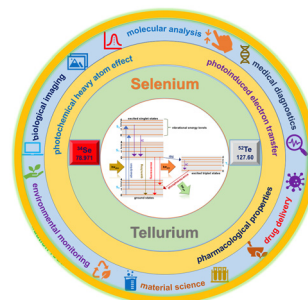
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Avtar Singh,* Jaspreet Dhau, Rajeev Kumar, Rahul Badru and Ajeet Kaushik



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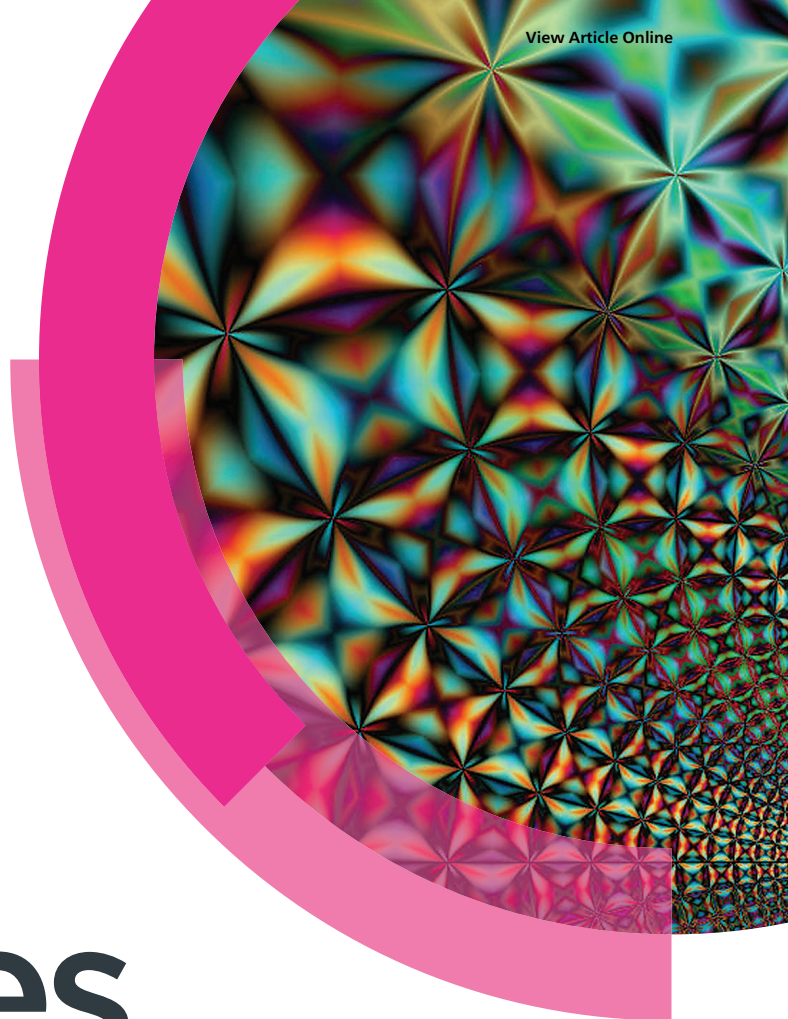


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Art, fact and artifact: reflections on the cross-talk between theory and experiment

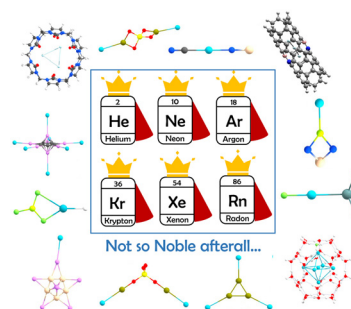
Judith Herzfeld



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Structure, stability, reactivity and bonding in noble gas compounds

Ranita Pal and Pratim Kumar Chattaraj*

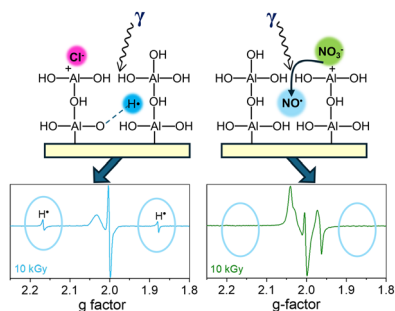


COMMUNICATION

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Effect of impurities on radical formation in gibbsite radiolysis

Hanna Hlushko, Alejandro Ramos-Ballesteros, Ping Chen, Xin Zhang, Kevin M. Rosso, Carolyn I. Pearce and Jay A. LaVerne*

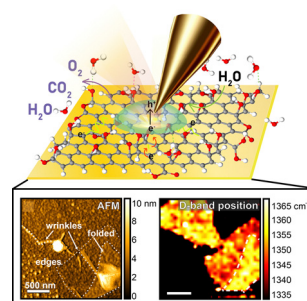


RESEARCH PAPERS

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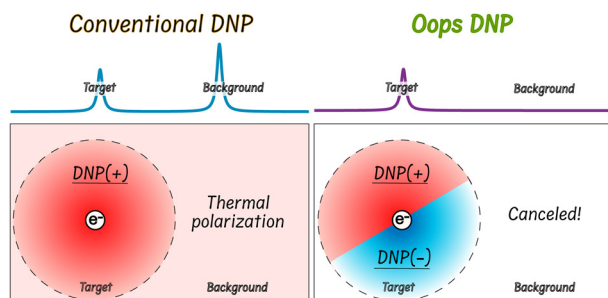
Nanoscale insights into graphene oxide reduction by tip-enhanced Raman spectroscopy

Xiao You,* Sangita Maharjan, Kizhanipuram Vinodgopal and Joanna M. Atkin*



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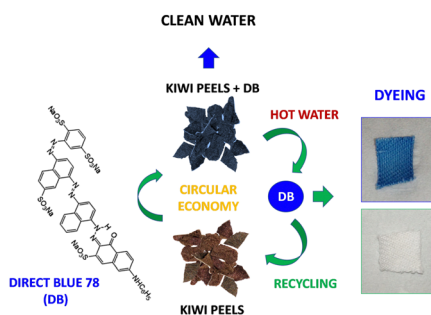
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Background signal suppression by opposite polarity subtraction for targeted DNP NMR spectroscopy on mixture samples

Zhongliang Zhang, Ken Kato, Hajime Tamaki and Yoh Matsuki*

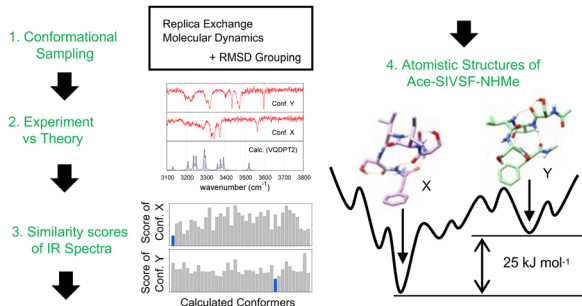
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Kiwi peel waste as a recyclable adsorbent to remove textile dyes from water: Direct Blue 78 removal and recovery

Jennifer Gubitosa, Vito Rizzi,* Paola Fini, Sergio Nuzzo and Pinalysa Cosma

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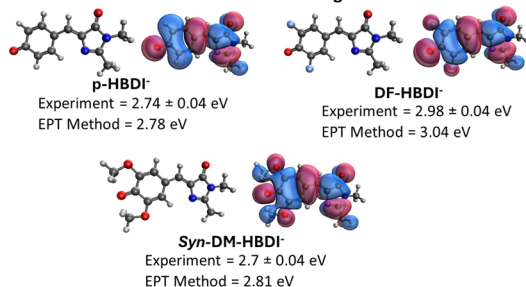


Similarity scores of vibrational spectra reveal the atomistic structure of pentapeptides in multiple basins

Hiroki Otaki, Shun-ichi Ishiuchi, Masaaki Fujii, Yuji Sugita and Kiyoshi Yagi*

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Lowest Vertical Electron Detachment Energies of GFP Model Anions



New-generation electron-propagator methods for vertical electron detachment energies of molecular anions: benchmarks and applications to model green-fluorescent-protein chromophores

Ernest Opoku, Filip Pawłowski and J. V. Ortiz*

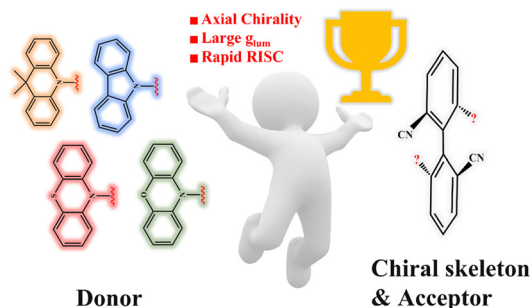


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Modulation of luminescence properties of circularly polarized thermally activated delayed fluorescence molecules with axial chirality by donor engineering

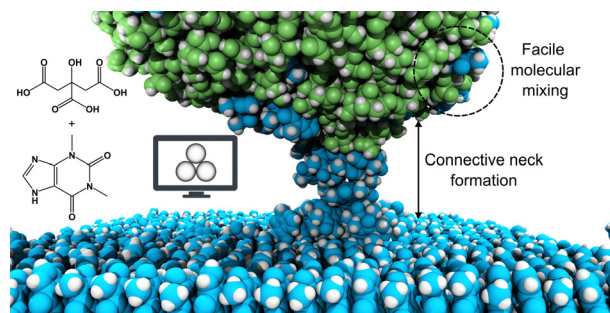
Shulei Liu, Songsong Liu, Yang Gao, Lili Lin,
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Exploring mechanochemistry of pharmaceutical cocrystals: effect of incident angle on molecular mixing during simulated indentations of two organic solids

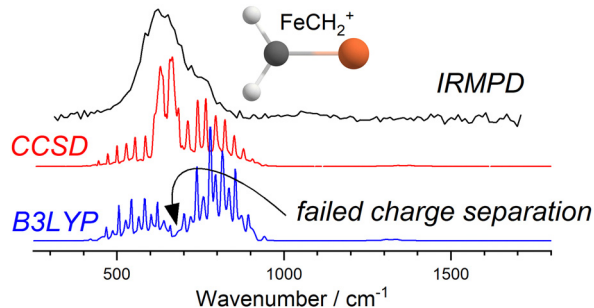
Michael Ferguson* and Tomislav Friščić*



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IR spectroscopic characterization of 3d transition metal carbene cations, FeCH_2^+ and CoCH_2^+ : periodic trends and a challenge for DFT approaches

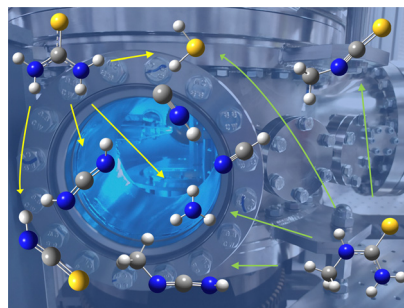
Frank J. Wensink, Corry E. Smink, P. B. Armentrout* and Joost M. Bakker*



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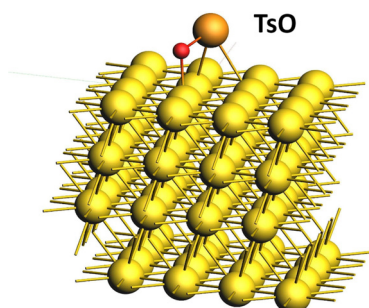
UV photolysis of thiourea and its *N*-methylated derivative in cryogenic matrices

Sándor Góbi,* Barbara Keresztes, Anita Schneiker and György Tarczay



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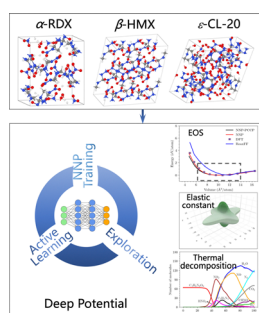
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Reactivity of Ts and At oxides and oxyhydrides with a gold surface from periodic DFT calculations

Anton Ryzhkov, Valeria Pershina, Miroslav Iliaš* and Vladimir Shabaev

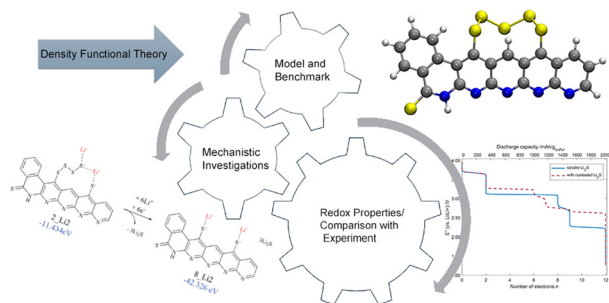
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Determining the mechanical and decomposition properties of high energetic materials (α -RDX, β -HMX, and ϵ -CL-20) using a neural network potential

Mingjie Wen, Xiaoya Chang, Yabei Xu, Dongping Chen and Qingzhao Chu*

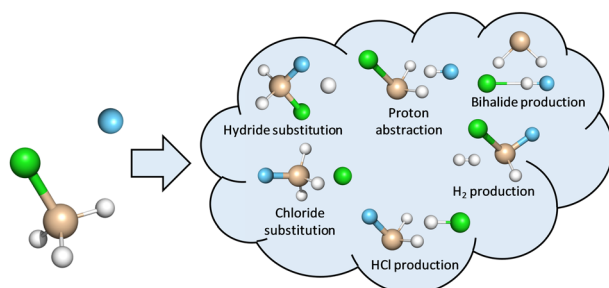
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The reduction behavior of sulfurized polyacrylonitrile (SPAN) in lithium-sulfur batteries using a carbonate electrolyte: a computational study

S. V. Klostermann, J. Kappler, A. Waigum, M. R. Buchmeiser, A. Köhn and J. Kästner*

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Detailed quasiclassical dynamics of the $F^- + SiH_3Cl$ multi-channel reaction

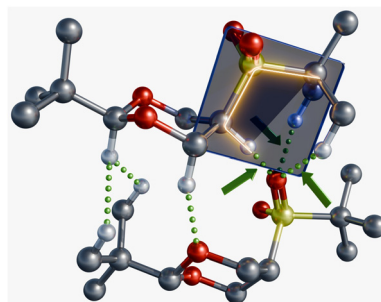
Attila Á. Dékány and Gábor Czakó*



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Stereoelectronic interactions are too weak to explain the molecular conformation in solid state of *cis*-2-*tert*-butyl-5-(*tert*-butylsulfonyl)-1,3-dioxane

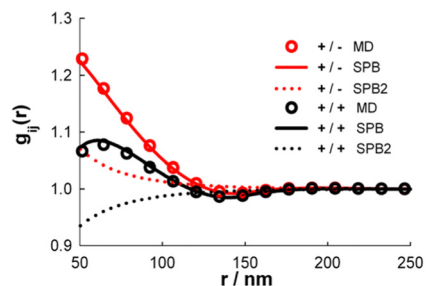
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Application of the symmetric Poisson–Boltzmann theory to a model colloidal mixture

Miguel Molero, Christopher W. Outhwaite and Lutful Bari Bhuiyan*

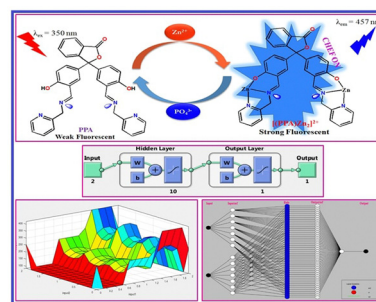


Theory vs simulations colloid / ion radial distribution functions

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A fluorescence based dual sensor for Zn^{2+} and PO_4^{3-} and the application of soft computing methods to predict machine learning outcomes

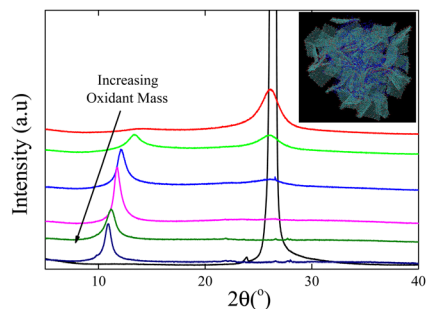
Shashanka Shekhar Samanta, Subhadip Giri, Sourav Mandal, Usha Mandal, Hasibul Beg and Ajay Misra*



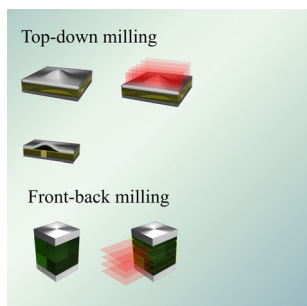
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Varying the degree of oxidation of graphite: effect of oxidation time and oxidant mass

Ioannis Karnis, Fanourios Krasanakis, Labrini Sygellou, Anastassia N. Rissanou, Konstantinos Karatasos and Kiriaki Chrissopoulou*



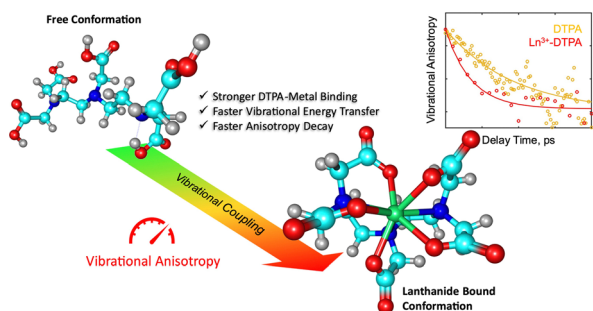
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Direct visualization and 3D reconstruction of conductive filaments in aSiO₂ material-based memristive device

Stanislav Slang, Bin Gu, Bo Zhang,* Petr Janicek, Jhonatan Rodriguez-Pereira and Tomas Wagner

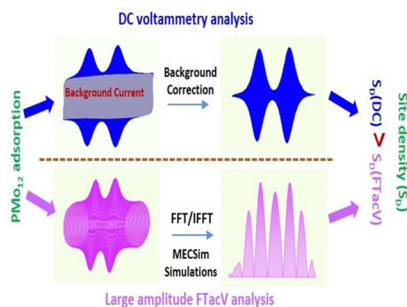
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Vibrational anisotropy decay resolves rare earth binding induced conformational change in DTPA

Ranadeb Ball, Jessica A. Jackson, Tomekia Simeon, George C. Schatz, Jenifer C. Shafer and Jessica M. Anna*

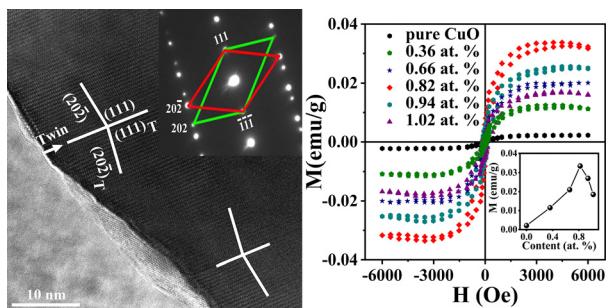
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Estimation of the electrochemical active site density of a metal-free carbon-based catalyst using phosphomolybdate (PMO₁₂) as an adsorbate

Rajan Maurya, Rubul Das, Shreya Sharma and Manoj Neergat*

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Structure-dependent spin-polarized electron transport in twin-crystal Cu_{1-x}Eu_xO semiconductors

Kewei Zhang, Xi Chen, Mingyan Chuai* and Mingzhe Zhang*

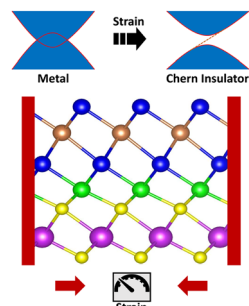


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Strain-induced topological phase transition in ferromagnetic Janus monolayer $\text{MnSbBiS}_2\text{Te}_2$

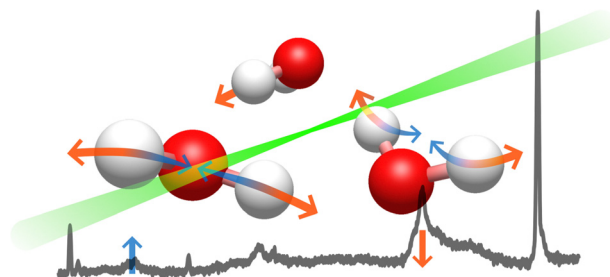
Romakanta Bhattarai, Peter Minch, Yunfan Liang, Shengbai Zhang and Trevor David Rhone*



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The strength of the OH-bend/OH-stretch Fermi resonance in small water clusters

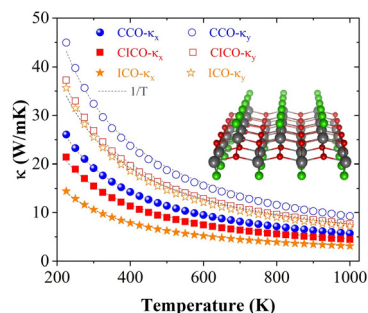
Nils O. B. Lüttschwager



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Investigation of the lattice thermal transport properties of Janus XCIO ($X = \text{Cr}, \text{Ir}$) monolayers by first-principles calculations

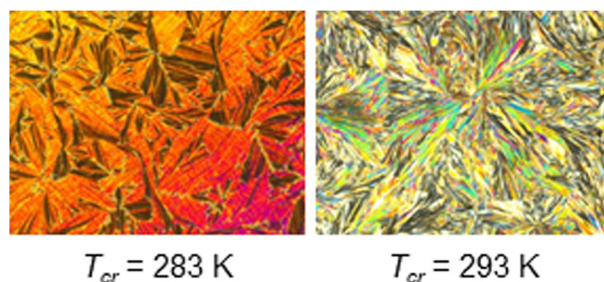
Peng Gao, Xihao Chen,* Zonghang Liu, Jiwen Li and Ning Wang*



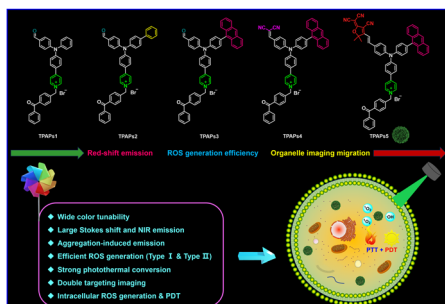
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Crystallization kinetics of (*S*)-4'-(1-methylheptyloxycarbonyl)biphenyl-4-yl 4-[4-(2,2,3,3,4,4,4-heptafluorobutoxy)but-1-oxy]-2-fluorobenzoate

Aleksandra Deptuch,* Sebastian Lalik, Małgorzata Jasiurkowska-Delaporte, Magdalena Urbańska and Monika Marzec

 $T_{cr} = 283 \text{ K}$ $T_{cr} = 293 \text{ K}$ 

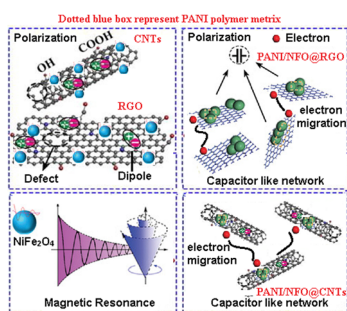
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Precise molecular engineering for the preparation of pyridinium photosensitizers with efficient ROS generation and photothermal conversion

Weidong Yin, Jianqing Li, Yucheng Ma, Weiqiang Li, Yanping Huo, Zujin Zhao* and Shaomin Ji*

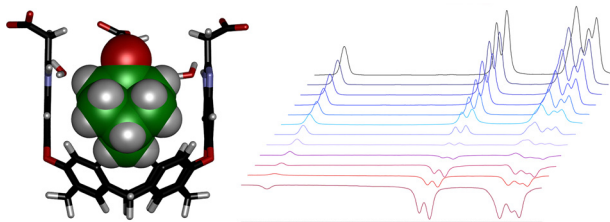
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Effect of carbon allotropes and thickness variation on the EMI shielding properties of PANI/NFO@CNTs and PANI/NFO@RGO ternary composite systems

Syeda Javaria Kazmi, Saeed Ur Rehman, M. Nadeem, Ubaid Ur Rehman, Shahzad Hussain* and Sadia Manzoor*

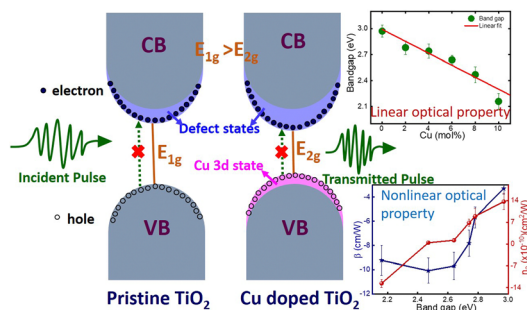
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Investigation of the effects on proton relaxation times upon encapsulation in a water-soluble synthetic receptor

Krishna N. Chaudhary, Kyra I. Brosnahan, Lucas J. Gibson-Elias, Jose L. Moreno Jr, Briana L. Hickey, Richard J. Hooley and Bethany G. Caulkins*

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Influence of defects on the linear and nonlinear optical properties of Cu-doped rutile TiO₂ microflowers

Subhashree Sahoo, Km. Surbhi, Sourav Bhakta, Ritwick Das and Pratap K. Sahoo*

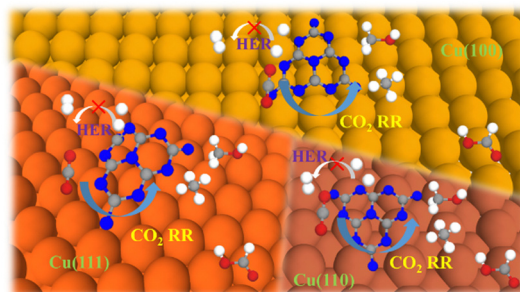


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Composite interfaces of g-C₃N₄ fragments loaded on a Cu substrate for CO₂ reduction

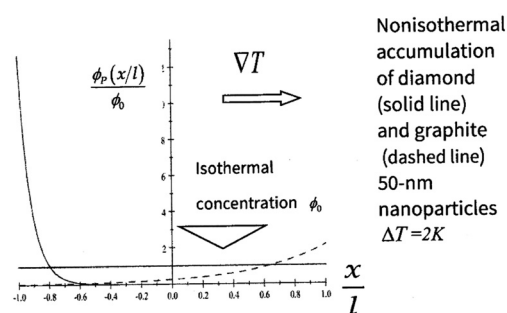
Qiang Gong, Jianling Xiong, Tanyu Zhou, Wenkai Bao, Xiuyun Zhang, Guiwu Liu,* Guanjun Qiao and Ziwei Xu*



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Phonon thermophoresis of crystalline nanoparticles in liquids

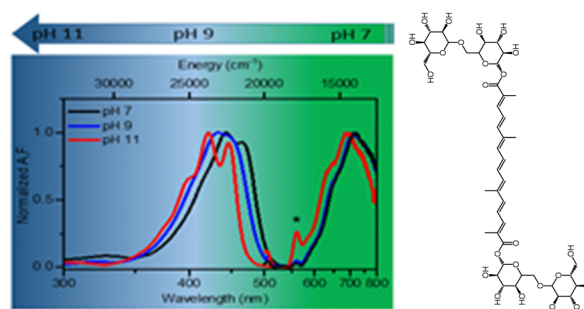
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Ultrafast spectroscopy of the hydrophilic carotenoid crocin at various pH

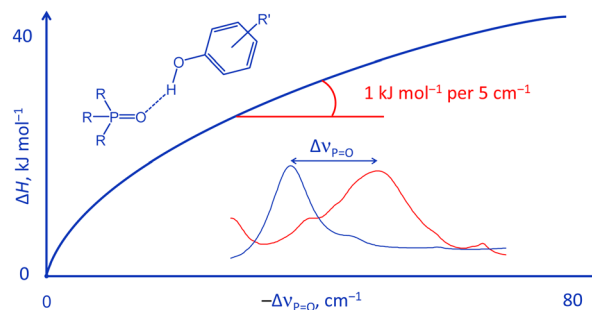
Emrah Özcan, Ivana Šimová, David Bina, Radek Litvín and Tomáš Polívka*



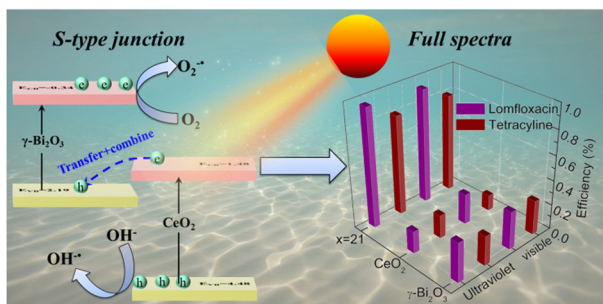
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Complexes of phosphine oxides with substituted phenols: hydrogen bond characterization based on shifts of P=O stretching bands

Mikhail A. Kostin, Omar Alkhuder, Luhang Xu, Danil V. Krutin, Ruslan E. Asfin* and Peter M. Tolstoy*



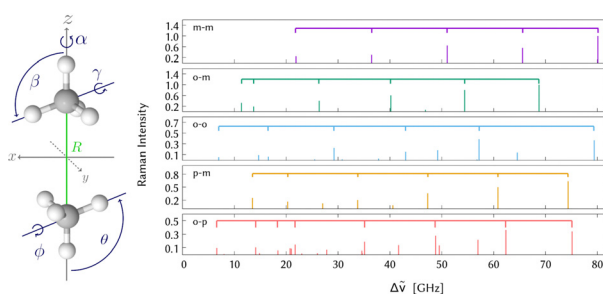
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Construction of a novel S-type $\gamma\text{-Bi}_2\text{O}_3/\text{CeO}_2$ heterojunction for highly efficient photocatalytic degradation of antibiotics

Jun Cao, Shuai Liu, Jiawei Wu, Bangfu Ding,* Liang Mao, Lei Zhang, Shukai Zheng and Junying Zhang

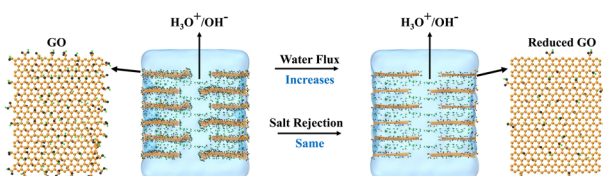
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Methane dimer rovibrational states and Raman transition moments

Alberto Martín Santa Daría, Gustavo Avila and Edit Mátyus*

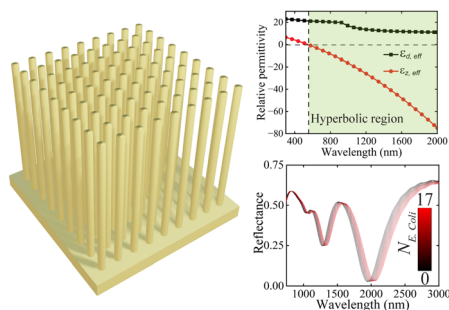
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Reduction-enhanced water flux through layered graphene oxide (GO) membranes stabilized with H_3O^+ and OH^- ions

Abhijit Gogoi,* Erik C. Neyts and François M. Peeters

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Titanium nitride-based hyperbolic metamaterial for near-infrared ultrasensitive sensing of microbes

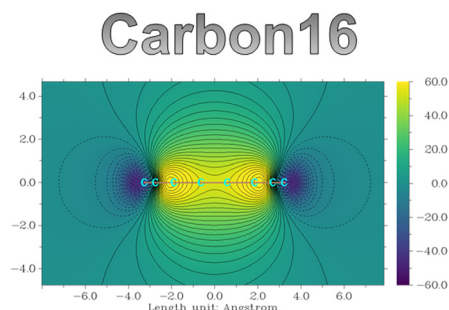
Dip Sarker and Ahmed Zubair*



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Theoretical insight into the doubly antiaromatic carbon allotrope cyclo[16]carbon

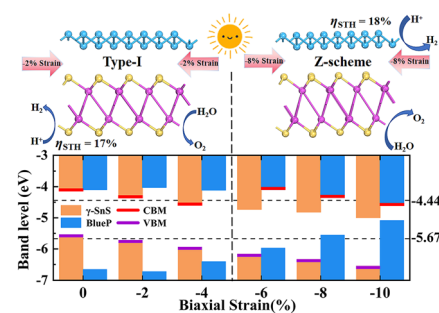
Hao Li, Rakesh Parida, Shaul Mukamel* and Jin Yong Lee*



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Strain-induced excellent photocatalytic performance in Z-scheme BlueP/ γ -SnS heterostructures for water splitting

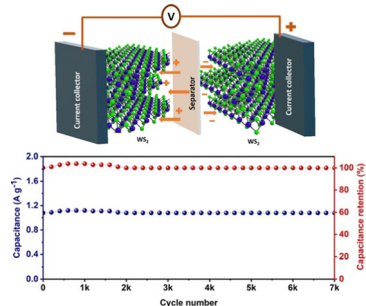
Quan Li, Jiabao Wang, Hao Huang, Guangting Zhao, Ling-Ling Wang and Xiaojun Zhu*



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Experimental and theoretical insights into the supercapacitive performance of interconnected WS₂ nanosheets

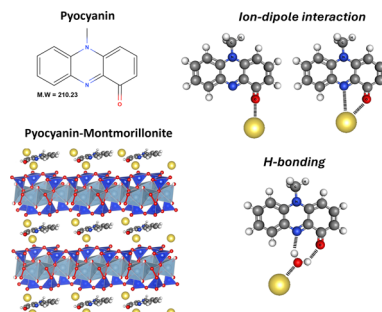
Shilpi Sengupta, Silda Peters, Tumpa Sadhukhan* and Manab Kundu*



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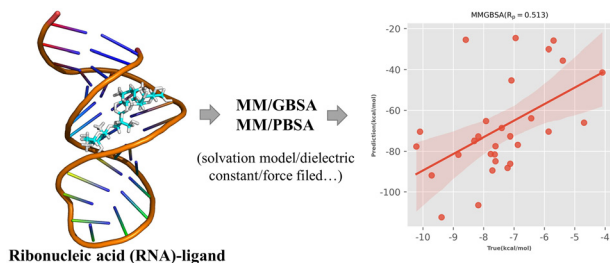
Insights on adsorption of pyocyanin in montmorillonite using molecular dynamics simulation

Bidemi Fashina,* Youjun Deng,* Tahir Cagin and Randall Cygan



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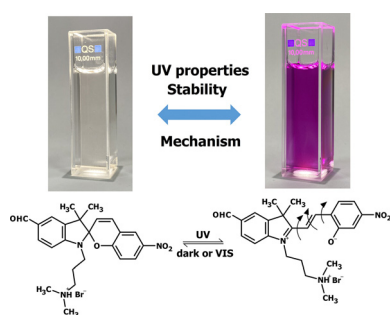
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Assessing the performance of MM/PBSA and MM/GBSA methods. 10. Prediction reliability of binding affinities and binding poses for RNA–ligand complexes

Dejun Jiang, Hongyan Du, Huifeng Zhao, Yafeng Deng, Zhenxing Wu, Jike Wang, Yundian Zeng, Haotian Zhang, Xiaorui Wang, Ercheng Wang,* Tingjun Hou* and Chang-Yu Hsieh*

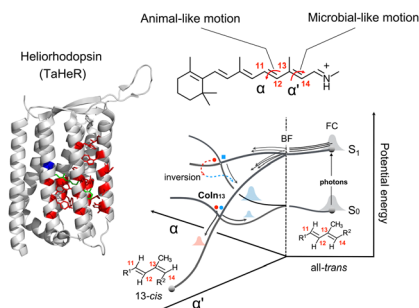
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Is this how bromine spiropyran salt is converted to merocyanine under UV irradiation? A look through the prism of quantum chemical calculations

Arthur R. Tulyabaev,* Artur A. Khuzin, Timur I. Lukmanov and Denis Sh. Sabirov

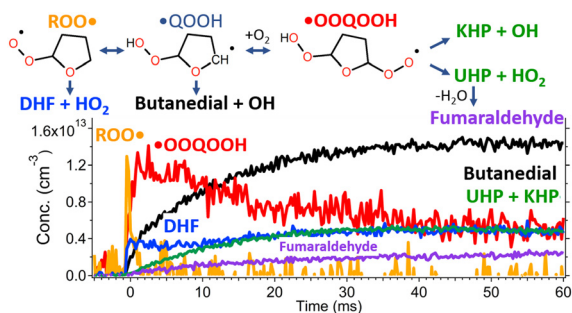
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Picosecond quantum-classical dynamics reveals that the coexistence of light-induced microbial and animal chromophore rotary motion modulates the isomerization quantum yield of heliorhodopsin

Riccardo Palombo, Leonardo Barneschi, Laura Pedraza-González, Xuchun Yang and Massimo Olivucci*

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Time-resolved quantification of key species and mechanistic insights in low-temperature tetrahydrofuran oxidation

Maria Demireva,* Kendrew Au, Nils Hansen and Leonid Sheps*

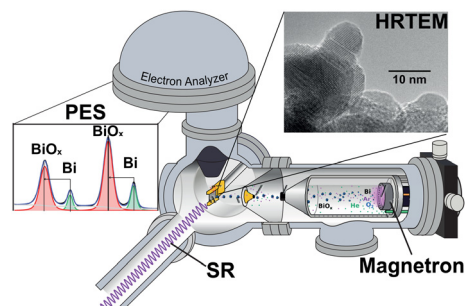


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Bismuth-oxide nanoparticles: study in a beam and as deposited

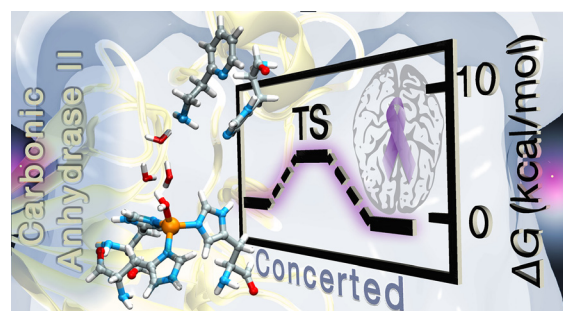
M.-H. Mikkela, M. Marnauza, C. J. D. Hetherington, R. Wallenberg, E. Märsell, Yen-Po Liu, A. Mikkelsen, O. Björneholm, G. Öhrwall and M. Tchaplyguine



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Insight into the activation mechanism of carbonic anhydrase(II) through 2-(2-aminoethyl)-pyridine: a promising pathway for enhanced enzymatic activity

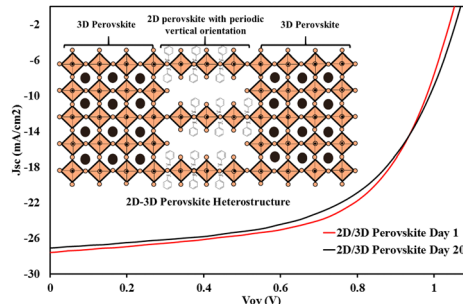
Masoumeh Shams Ghamsary, Mina Ghiasi* and S. Shahab Naghavi*



10392

A bromide substituted 2D additive for stable and efficient perovskite photovoltaics

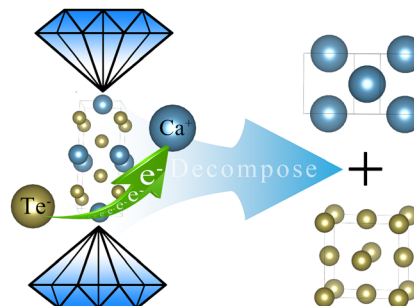
Muhammad Sohail Abbas,* Sabir Hussain, Jianqi Zhang, Boxin Wang, Zhen Wang, Chen Yang and Rashid Ahmad*



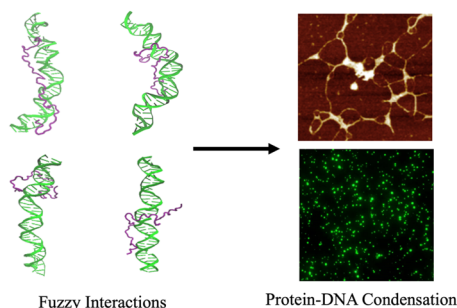
10399

Reverse charge transfer and decomposition in Ca–Te compounds under high pressure

Yang Lv, Jianfu Li,* Zhaobin Zhang, Yanlei Geng, Zhenzhen Xu, Yong Liu, Jianan Yuan, Qinglin Wang and Xiaoli Wang*



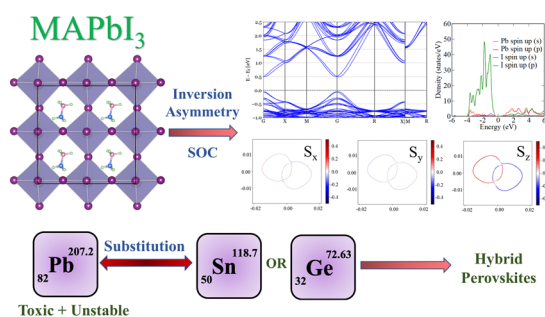
10408



Probing the hierarchical dynamics of DNA-sperm nuclear transition protein complexes through fuzzy interaction and mesoscale condensation

Shangqiang Xie, Congran Yue, Sheng Ye* and Zhenlu Li*

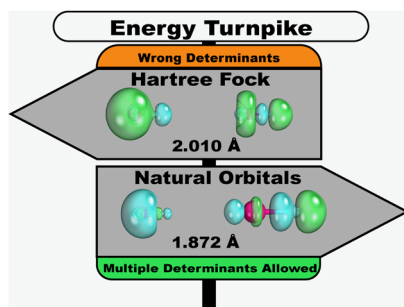
10419



Rashba and Dresselhaus effects in doped methylammonium lead halide perovskite MAPbI₃

Megha Arya, Preeti Bhumla, Sajjan Sheoran and Saswata Bhattacharya*

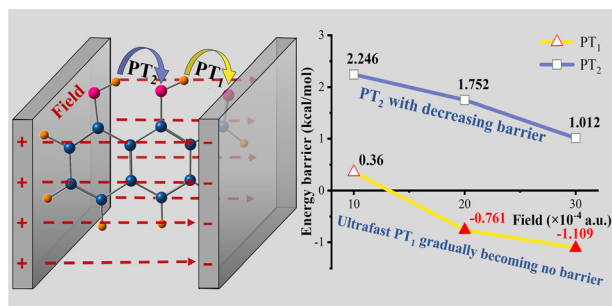
10427



Unraveling the electronic structure of LuH, LuN, and LuNH: building blocks of new materials

Nuno M. S. Almeida, Bradley K. Welch, Sasha C. North and Angela K. Wilson*

10439



Effect of external electric fields on the ESDPT process and photophysical properties of 1,8-dihydroxy-2-naphthaldehyde

Xingzhu Tang, Yajie Zhang and Chaofan Sun*

