

IN THIS ISSUE

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Inside cover

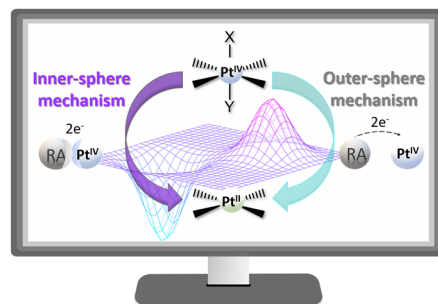
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PERSPECTIVES

15586

The current status in computational exploration of Pt(IV) prodrug activation by reduction

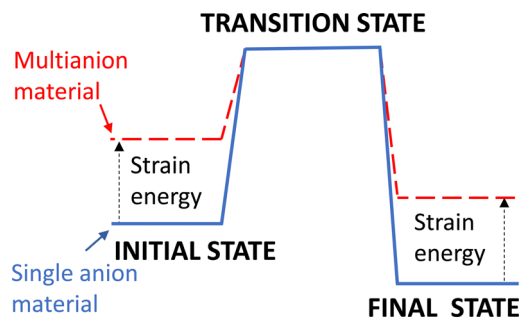
Fortuna Ponte, Stefano Scoditti, Gloria Mazzone* and Emilia Sicilia*



15600

New perspectives on the multianion approach to adapt electrode materials for lithium and post-lithium batteries

Carlos Pérez-Vicente and Ricardo Alcántara*



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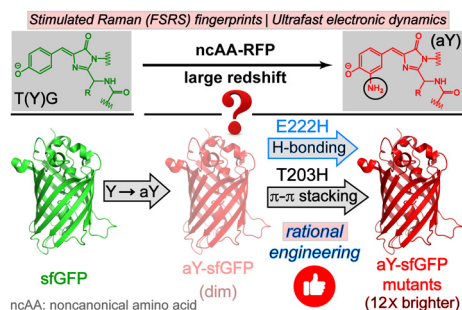


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15624

Structural origin and rational development of bright red noncanonical variants of green fluorescent protein

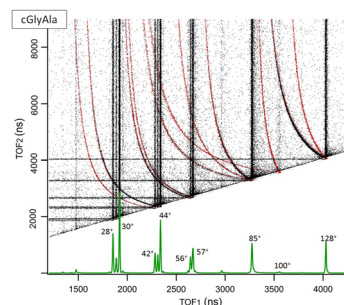
Cheng Chen, Hao Zhang, Jing Zhang, Hui-wang Ai* and Chong Fang*



15635

Photofragmentation specificity of photoionized cyclic amino acids (diketopiperazines) as precursors of peptide building blocks

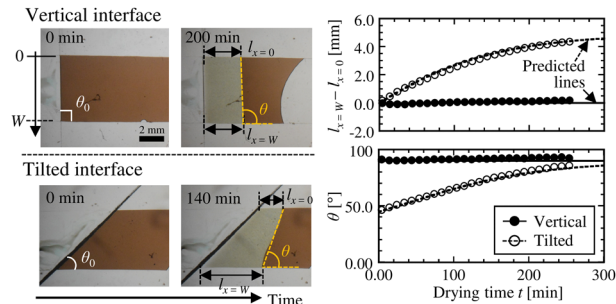
Dario Barreiro-Lage,* Jacopo Chiarinelli, Paola Bolognesi,* Robert Richter, Henning Zettergren, Mark H. Stockett, Sergio Díaz-Tendero and Lorenzo Avaldi



15647

Position-dependent rates of film growth in drying colloidal suspensions on tilted air–water interfaces

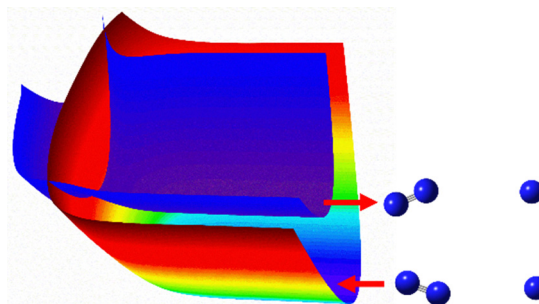
Kohei Abe* and Susumu Inasawa*



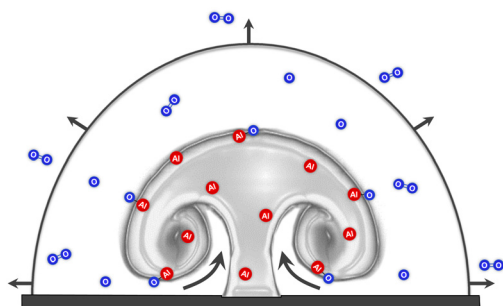
15656

Quantum and semiclassical studies of nonadiabatic electronic transitions between $N(^4S)$ and $N(^2D)$ by collisions with N_2

Dandan Lu, Breno R. L. Galvão, Antonio J. C. Varandas and Hua Guo*



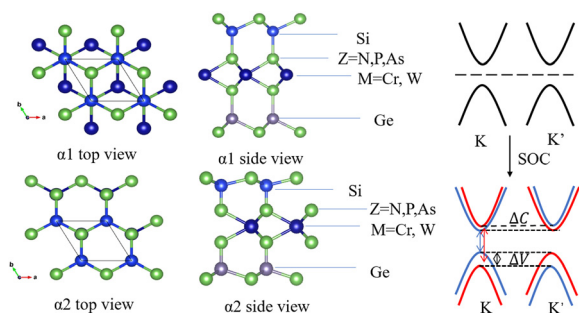
15666



Experimental and computational investigation into the hydrodynamics and chemical dynamics of laser ablation aluminum plasmas

Emily H. Kwapis,* Jacob W. Posey, Enrique Medici, Kira Berg, Ryan W. Houim and Kyle C. Hartig

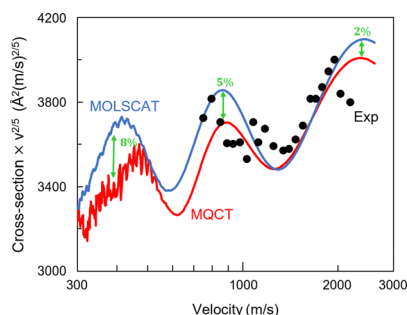
15676



Theoretical prediction of valley spin splitting in two-dimensional Janus MSiGeZ₄ (M = Cr and W; Z = N, P, and As)

Ying Li, Mengxian Lan, Suen Wang, Tian Huang, Yu Chen, Hong Wu, Feng Li* and Yong Pu*

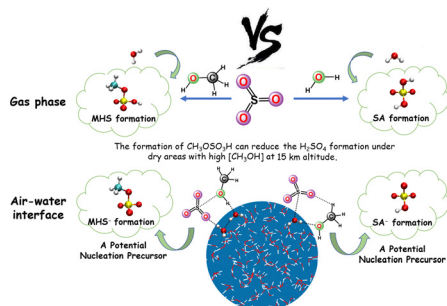
15683



Description of quantum interference using mixed quantum/classical theory of inelastic scattering

Dulat Bostan, Bikramaditya Mandal, Carolin Joy and Dmitri Babikov*

15693



Determination of the influence of water on the SO₃ + CH₃OH reaction in the gas phase and at the air–water interface

Chao Ding, Yang Cheng, Hui Wang, Jihuan Yang, Zeyao Li, Makroni Lily,* Rui Wang and Tianlei Zhang*

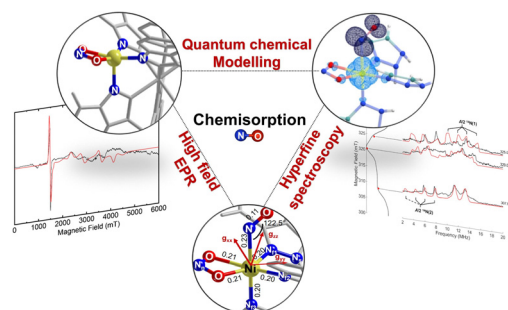


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15702

Unveiling the atomistic and electronic structure of Ni^{II}–NO adduct in a MOF-based catalyst by EPR spectroscopy and quantum chemical modelling

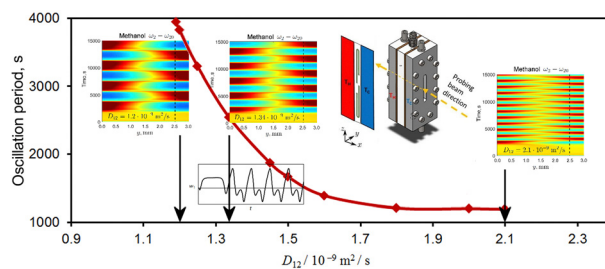
Kavipriya Thangavel, Paolo Cleto Bruzzese, Matthias Mendt, Andrea Folli, Katharina Knippen, Dirk Volkmer, Damien M. Murphy and Andreas Pöpl^{*}



15715

Cross diffusion governs an oscillatory instability in a ternary mixture with the Soret effect

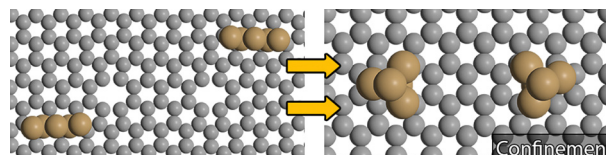
Berin Seta, Ane Errarte, Aliaksandr Mialdun, Ilya I. Ryzhkov, Mounir M. Bou-Ali and Valentina Shevtsova^{*}



15729

Carbon vacancy-assisted stabilization of individual Cu₅ clusters on graphene. Insights from *ab initio* molecular dynamics

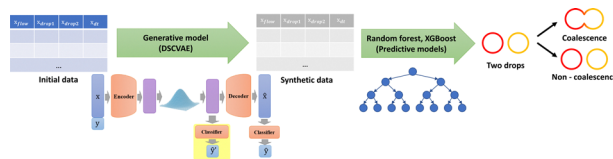
Lenard L. Carroll, Lyudmila V. Moskaleva^{*} and Maria Pilar de Lara-Castells^{*}



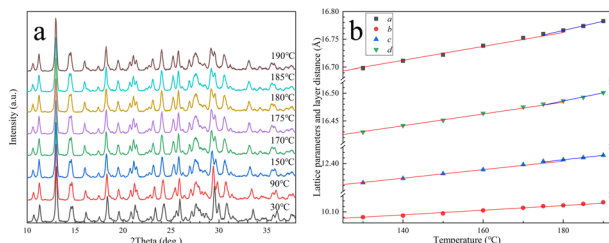
15744

Analyzing drop coalescence in microfluidic devices with a deep learning generative model

Kewei Zhu, Sib0 Cheng,^{*} Nina Kovalchuk, Mark Simmons, Yi-Ke Guo, Omar K. Matar and Rossella Arcucci



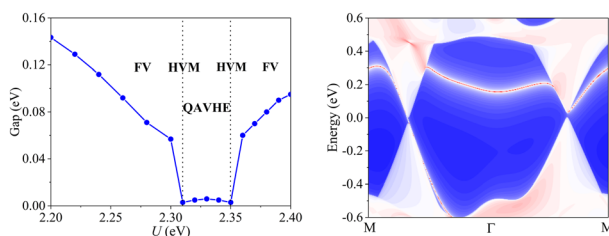
15756



Isothermal structural evolution of CL-20/HMX cocrystals under slow roasting at 190 °C

Wentao Liang, Xiaoyu Sun, He Wang, Junke Wang, Zhilei Sui, Haichao Ren, Rucheng Dai, Xianxu Zheng, Zhongping Wang,* Xiaohui Duan* and Zengming Zhang*

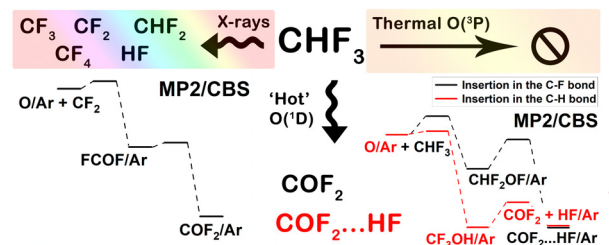
15767



Electronic-correlation induced sign-reversible Berry phase and quantum anomalous valley Hall effects in Janus monolayer OsClBr

Kang Jia, Xiao-Jing Dong, Sheng-Shi Li, Wei-Xiao Ji and Chang-Wen Zhang*

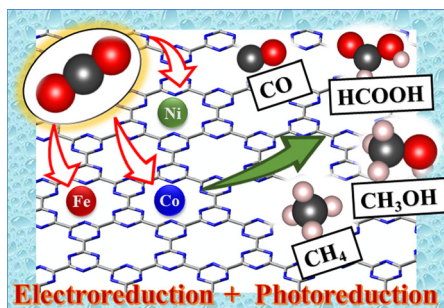
15777



Reactions of oxygen atoms with fluoroform and its radiolysis products: matrix isolation and *ab initio* study

Ilya S. Sosulin, Ekaterina S. Shiryayeva, Daniil A. Tyurin and Vladimir I. Feldman*

15788



Boosting photo-assisted efficient electrochemical CO₂ reduction reaction on transition metal single-atom catalysts supported on the C₆N₆ nanosheet

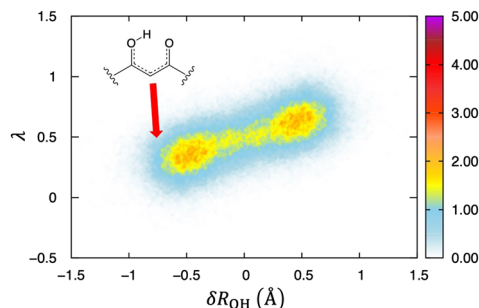
Supriti Dutta and Swapan K. Pati*



15798

Nuclear quantum and H/D isotope effects on intramolecular hydrogen bond in curcumin

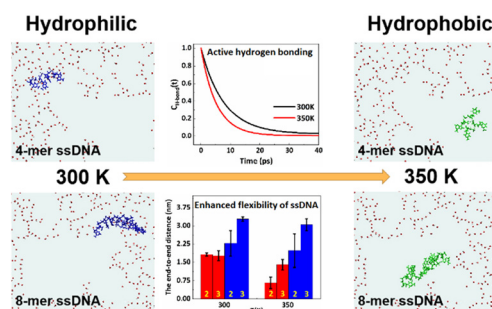
Taro Udagawa,* Hinata Yabushita, Hikaru Tanaka, Kazuaki Kuwahata and Masanori Tachikawa



15807

Dynamic behavior of the single-strand DNA molecules from the hydrophilic to hydrophobic regions on graphene oxide surface driven by heating

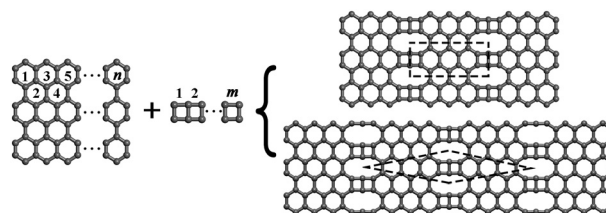
Mengjiao Wu, Yingying Huang, Li Yang, Yongshun Song* and Xiaoling Lei*



15815

A series of two-dimensional carbon allotropes with Dirac cone structure

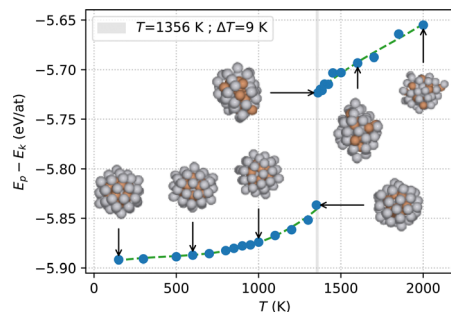
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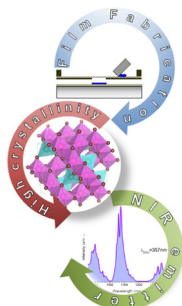
15822

Melting of FePt nanoparticles studied using DFT

Paweł T. Jochym,* Jan Łażewski and Przemysław Piekarczyk



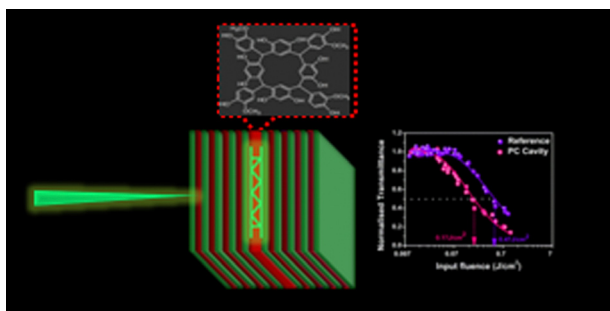
15829



Cost-effective screen printing approach for Ce/Nd-doped ZnAl₂O₄ films: tuning crystallinity induced by the substrate

Rocio E. Rojas-Hernandez,* Fernando Rubio-Marcos, Jallouli Necib, Mati Danilson, José F. Fernandez and Irina Hussainova

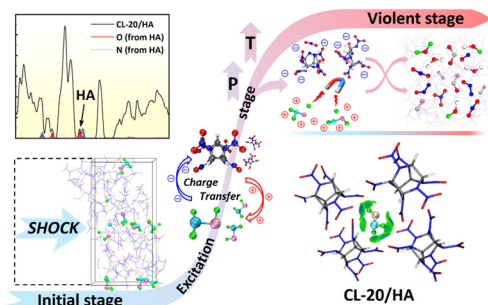
15839



Photonic crystal cavity-mediated improved absorptive nonlinearity of C-4-hydroxy-3-methoxyphenilcalix[4]resorcinarene

Siji Alappattu John, Athulya Kadeprath Satheesan, Simi Pushpan K. and Chandrasekharan Keloth*

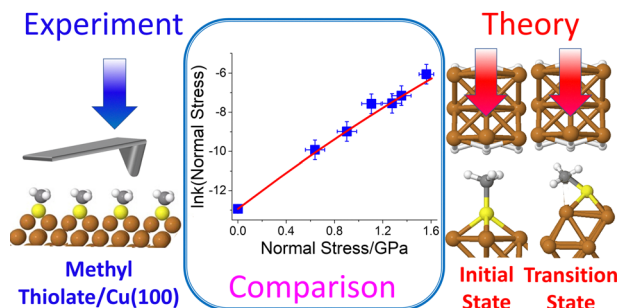
15846



Reaction mechanism and electronic properties of host-guest energetic material CL-20/HA under high pressure by quantum-based molecular dynamics simulations

Yiwen Xiao, Lang Chen,* Kun Yang, Jianying Lu and Junying Wu

15855



Exploring mechanochemical reactions at the nanoscale: theory versus experiment

Nicholas Hopper, François Sidoroff, Resham Rana, Robert Bavisotto, Juliette Cayer-Barrioz, Denis Mazuyer and Wilfred T. Tysoe*

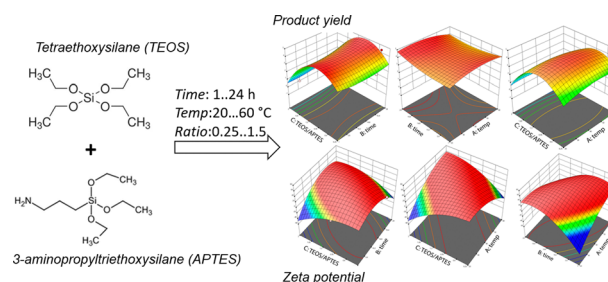


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15862

A statistical design approach to the sol–gel synthesis of (amino)organosilane hybrid nanoparticles

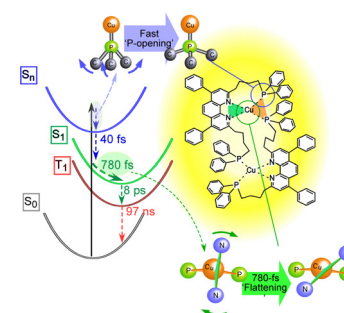
Lyubov Bondarenko,* Yaroslav Saveliev, Dmitry Chernyaev, Rose Baimuratova, Gulzhian Dzhardimalieva, Artur Dzeranov, Elena Kelbysheva and Kamila Kydralieva



15873

Structural change dynamics of heteroleptic Cu(i) complexes observed by ultrafast emission spectroscopy

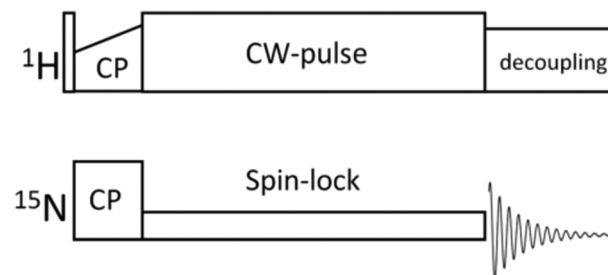
Masashi Sanga, Kosuke Nakamura, Munetaka Iwamura,* Koichi Nozaki, Hiroyuki Takeda,* Yu Monma and Osamu Ishitani



15885

Rocking motion in solid proteins studied by the ¹⁵N proton-decoupled R_{1ρ} relaxometry

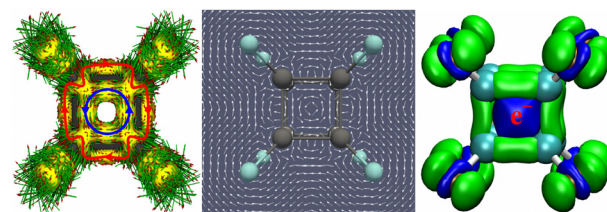
Alexey Krushelnitsky,* Günter Hempel, Hannes Jurack and Tiago Mendes Ferreira



15897

Bonding character, electronic properties, and electronic transitions of perfluorocubane as a small electron acceptor

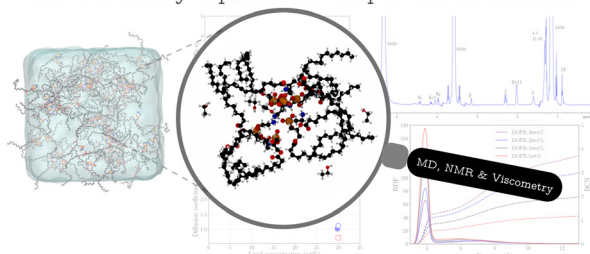
Xiaojun Li,* Shuna Li, Jun Lu, Hongjiang Ren, Mengqi Zhang and Wangdi Zhang



RESEARCH PAPERS

15905

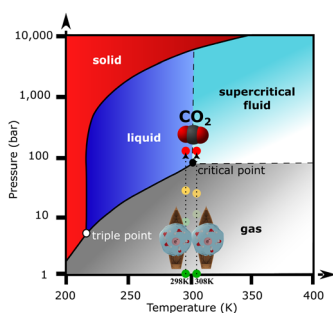
Simulation insight and interpretation of results from NMR and viscometry experiments in lipid-ethanol mixtures



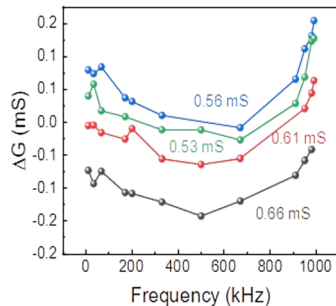
Phase equilibrium, dynamics and rheology of phospholipid-ethanol mixtures: a combined molecular dynamics, NMR and viscometry study

Fredrik Grote, Alexander Lyubartsev,*
Sergey V. Dvinskikh, Vibhu Rinwa and Jan Holmbäck

15916

Reactivity of presolvated and solvated electrons with CO₂ in water up to 118 bar at 298 and 308 KDenis S. Dobrovolskii, Mehran Mostafavi and
Sergey A. Denisov*

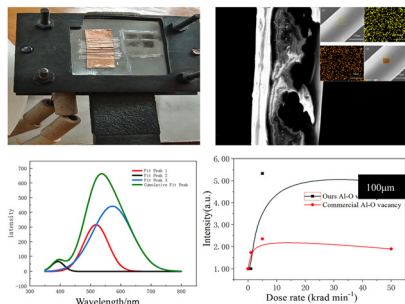
15920



Tuning Bienenstock-Cooper-Munro learning rules in a two-terminal memristor for neuromorphic computing

Zeyang Li, Peilin Liu, Guanghong Yang, Caihong Jia* and
Weifeng Zhang*

15929



Promotional effects of cerium in ytterbium doped fibers on proton irradiation damage

Yang Shao, Yuting Wang* and Xin Ju*

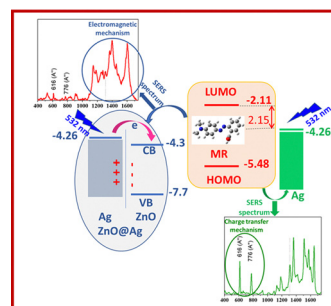


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15941

Enhanced Raman scattering based on a ZnO/Ag nanostructured substrate: an in-depth study of the SERS mechanism

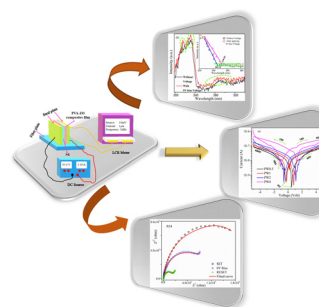
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15953

Tunable, reversible resistive switching behavior of PVA-zirconia nanocomposite films and validation of the trap-assisted switching mechanism by the selective application of external bias voltages

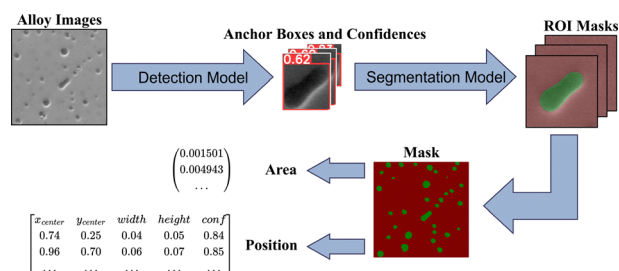
Riju Karmakar, Amit Kumar Das, Bilwadal Dutta, Subhojyoti Sinha,* Saikat Santra, Subhamay Pramanik, Probooth Kumar Kuri and Ajit Kumar Meikap*



15970

Accurate identification and measurement of the precipitate area by two-stage deep neural networks in novel chromium-based alloys

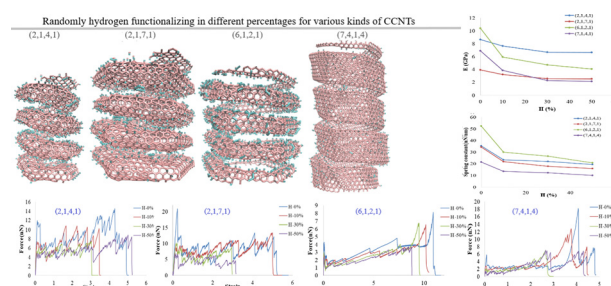
Zeyu Xia, Kan Ma, Sibao Cheng,* Thomas Blackburn, Ziling Peng, Kewei Zhu, Weihang Zhang, Dunhui Xiao, Alexander J Knowles and Rossella Arcucci



15988

Unraveling the effect of hydrogenation on the mechanical properties of coiled carbon nanotubes: a molecular dynamics study

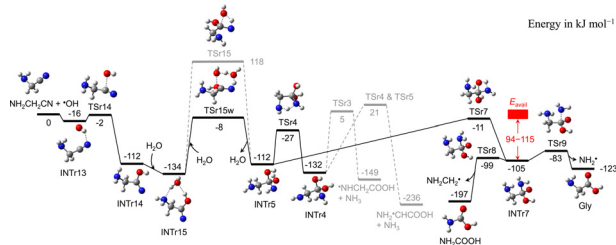
Mahdi Azhari Saray, Mostafa Baghani, Ali Rajabpour, Ali Sharifian* and Majid Baniassadi*



16001

Mechanisms of glycine formation from aminoacetonitrile in space

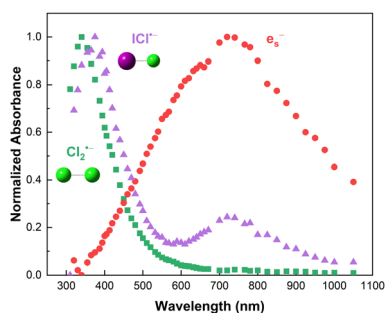
Joong Chul Choe



16009

Impact of iodide ions on the speciation of radiolytic transients in molten LiCl–KCl eutectic salt mixtures

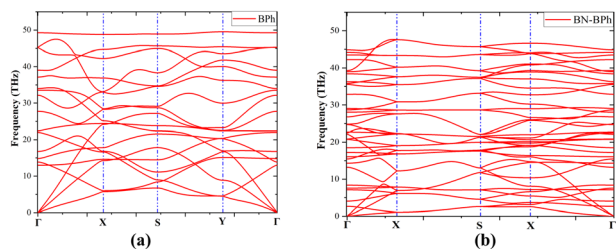
Jacy K. Conrad,* Kazuhiro Iwamatsu, Michael E. Woods, Ruchi Gakhar, Bobby Layne, Andrew R. Cook and Gregory P. Horne*



16018

2D BN-biphenylene: structure stability and properties tenability from a DFT perspective

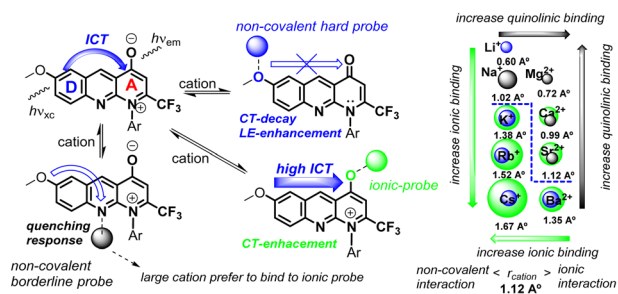
Mukesh Singh and Brahmananda Chakraborty*



16030

Exploring binding chemistry of alkali/alkaline earth cations in solution through modulation of intramolecular charge-transfer in an excited ambidentate organic fluorophore

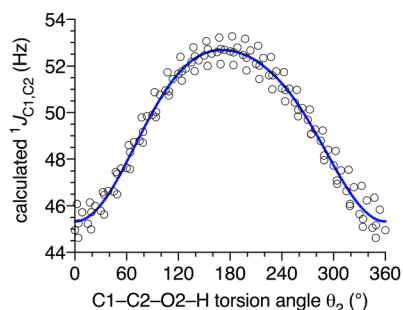
Angel H. Romero,* Lourdes Gotopo, Gustavo Cabrera and Hugo Cerecetto



16048

One-bond ^{13}C – ^{13}C spin-coupling constants in saccharides: a comparison of experimental and calculated values by density functional theory using solid-state ^{13}C NMR and X-ray crystallography

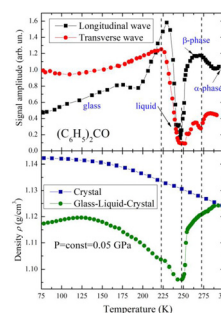
Timothy Tetrault, Reagan J. Meredith, Mi-Kyung Yoon, Christopher Canizares, Allen G. Oliver, Ian Carmichael and Anthony S. Serianni*



16060

Benzophenone glass, supercooled liquid, and crystals: elastic properties and phase transitions

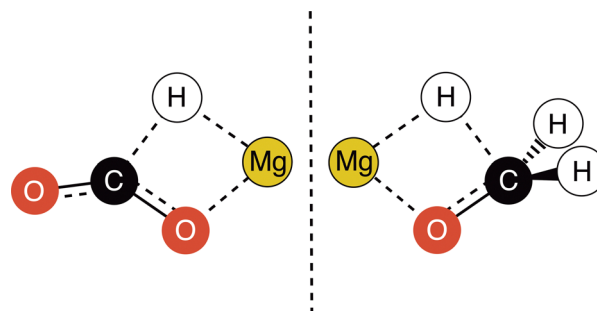
Elena L. Gromnitskaya,* Igor V. Danilov, Fedor I. Zubkov and Vadim V. Brazhkin



16065

Gas phase models of hydride transfer from divalent alkaline earth metals to CO_2 and CH_2O

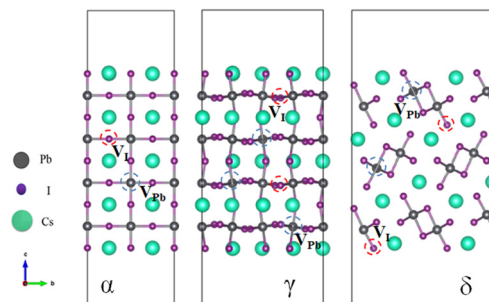
Christian Sant Gjermestad, Mauritz Johan Ryding and Einar Uggerud*



16077

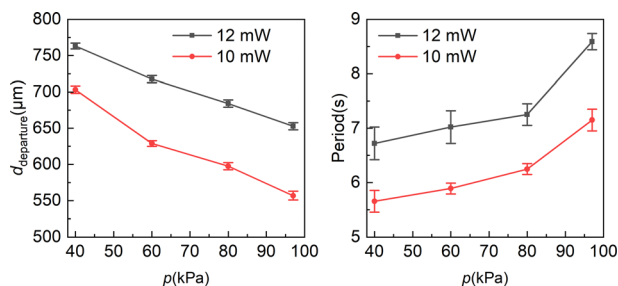
Intrinsic defects on α , γ and δ - CsPbI_3 (001) surfaces and implications for the α/γ to δ phase transition

Na Wang* and Yaqiong Wu



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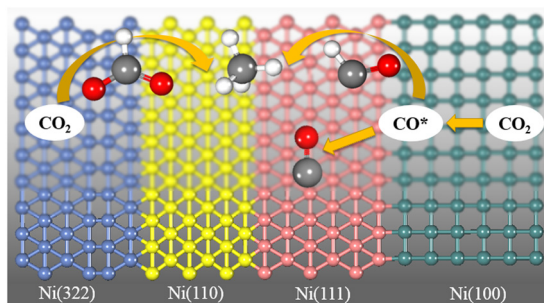
16086



Influence of subatmospheric pressure on bubble evolution on the TiO_2 photoelectrode surface

Xinyi Luo, Qiang Xu,* Tengfei Nie, Yonglu She, Xingmiao Ye and Liejin Guo

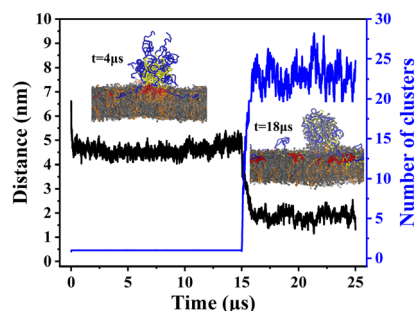
16105



Meso-scale study of crystal-plane effects of Ni catalysts on CO_2 hydrogenation

Xiaolei Wang, Ning Liu, Ruinian Xu, Biaohua Chen,* Chengna Dai and Gangqiang Yu

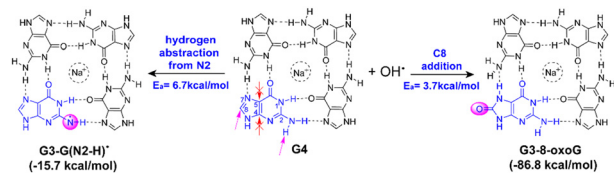
16114



Delivery mechanism of doxorubicin by PEG- DPPE micelles on membrane invasion by dynamic simulations

Lina Zhao, Meina Ren, Yanjiao Wang, Hailong An* and Fude Sun*

16126



Theoretical insights into the reaction mechanism of hydroxyl radicals and guanine in G-quadruplex DNA

Yinghui Wang* and Simin Wei*

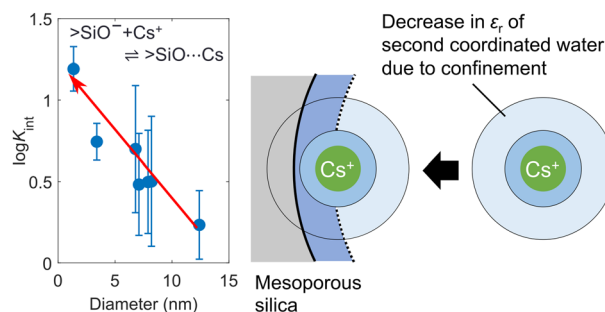


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16135

Adsorption of cesium and strontium on mesoporous silicas

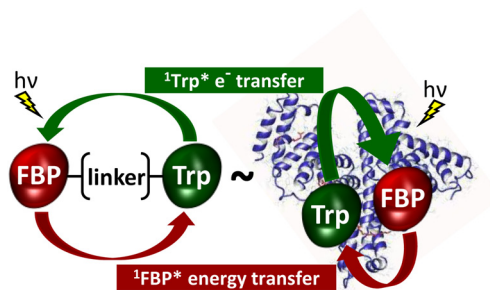
Kento Murota,* Yoshio Takahashi and Takumi Saito



16148

Topological effects in ultrafast photoinduced processes between flurbiprofen and tryptophan in linked dyads and within human serum albumin

Lorena Tamarit, Laura García-Gabarda, M. Consuelo Jiménez, Miguel A. Miranda* and Ignacio Vayá*



CORRECTION

16157

Correction: Helium nanodroplets as an efficient tool to investigate hydrogen attachment to alkali cations

Siegfried Kollotzek,* José Campos-Martínez,* Massimiliano Bartolomei, Fernando Pirani, Lukas Tiefenthaler, Marta I. Hernández, Teresa Lázaro, Eva Zunzunegui-Bru, Tomás González-Lezana, José Bretón, Javier Hernández-Rojas, Olof Echt and Paul Scheier

