

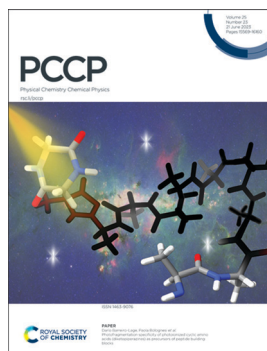
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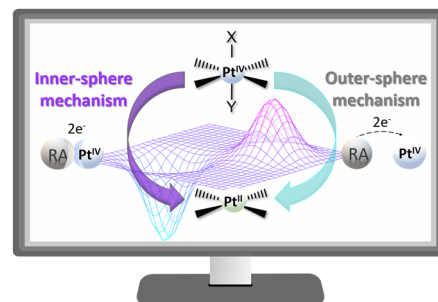
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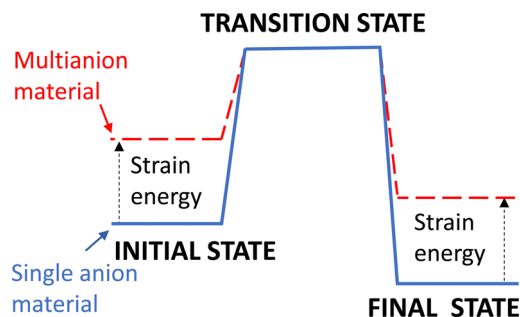
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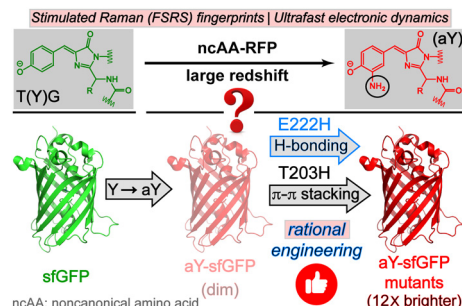


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# Structural origin and rational development of bright red noncanonical variants of green fluorescent protein

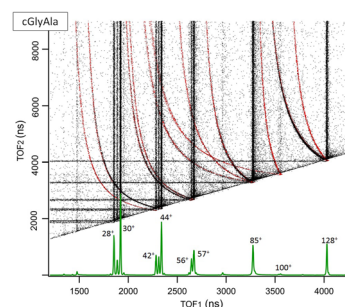
Cheng Chen, Hao Zhang, Jing Zhang, Hui-wang Ai\* and Chong Fang\*



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

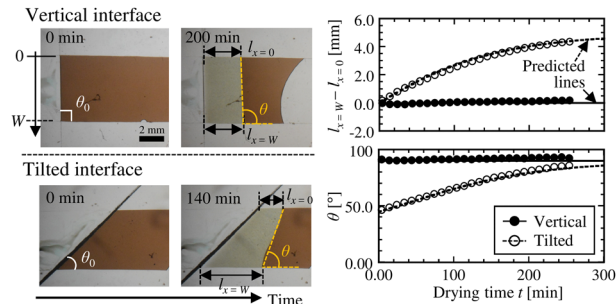
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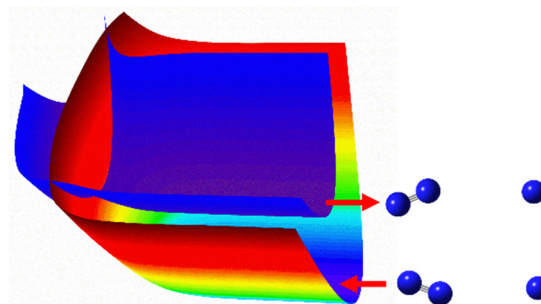
Kohei Abe\* and Susumu Inasawa\*



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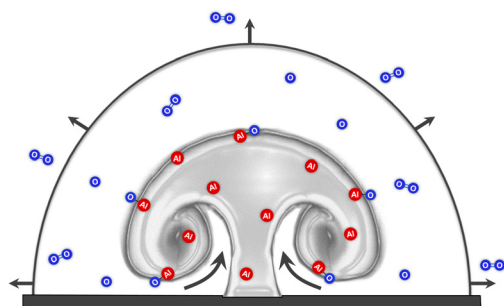
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Dandan Lu, Breno R. L. Galvão, Antonio J. C. Varandas and Hua Guo\*



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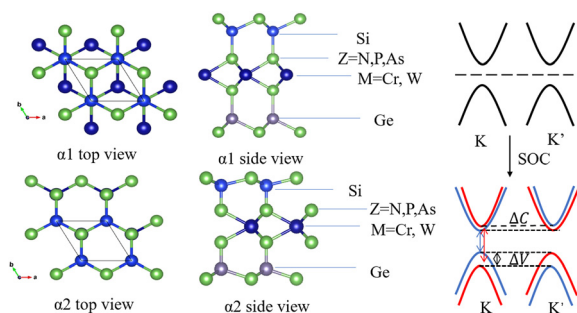
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### Experimental and computational investigation into the hydrodynamics and chemical dynamics of laser ablation aluminum plasmas

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

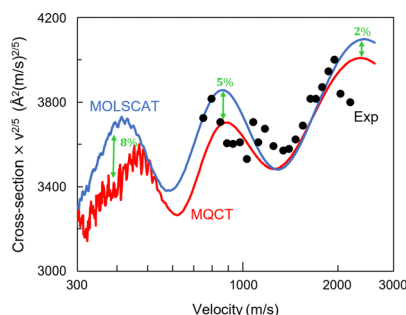
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### Theoretical prediction of valley spin splitting in two-dimensional Janus MSiGeZ<sub>4</sub> (M = Cr and W; Z = N, P, and As)

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

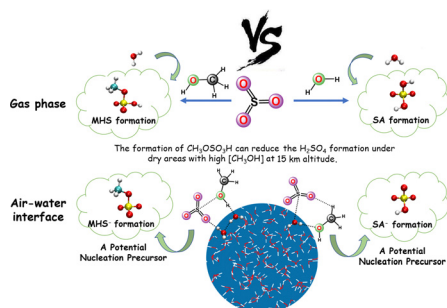
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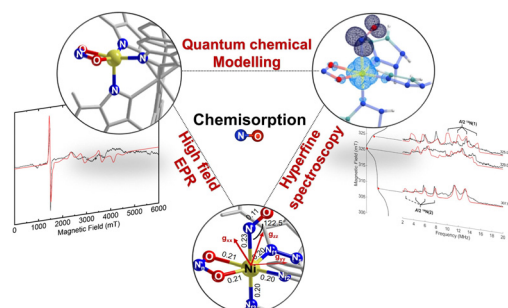


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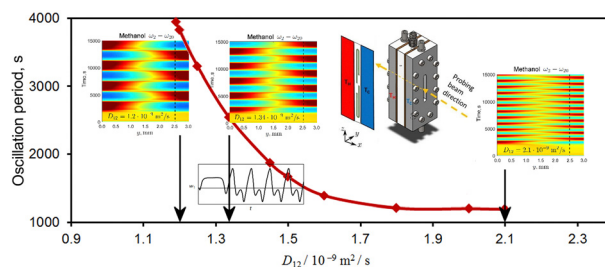
Kavipriya Thangavel, Paolo Cleto Bruzzese, Matthias Mendt, Andrea Folli, Katharina Knippen, Dirk Volkmer, Damien M. Murphy and Andreas Pöppel\*



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

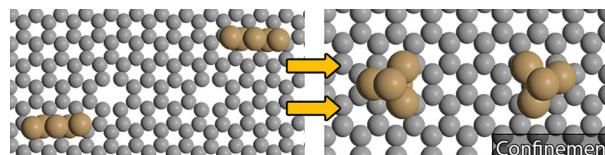
Berin Seta, Ane Errarte, Aliaksandr Mialdun, Ilya I. Ryzhkov, Mounir M. Bou-Ali and Valentina Shevtsova\*



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# Carbon vacancy-assisted stabilization of individual Cu<sub>5</sub> clusters on graphene. Insights from *ab initio* molecular dynamics

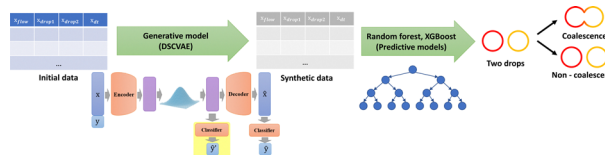
Lenard L. Carroll, Lyudmila V. Moskaleva\* and Maria Pilar de Lara-Castells\*



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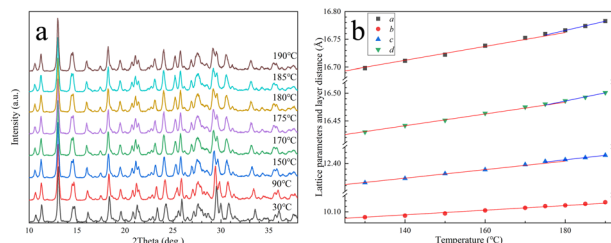
# Analyzing drop coalescence in microfluidic devices with a deep learning generative model

Kewei Zhu, Sibio Cheng,\* Nina Kovalchuk, Mark Simmons, Yi-Ke Guo, Omar K. Matar and Rossella Arcucci





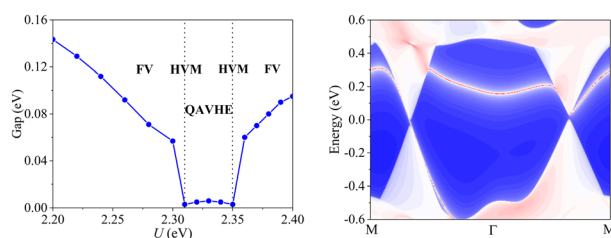
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### Isothermal structural evolution of CL-20/HMX cocrystals under slow roasting at 190 °C

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

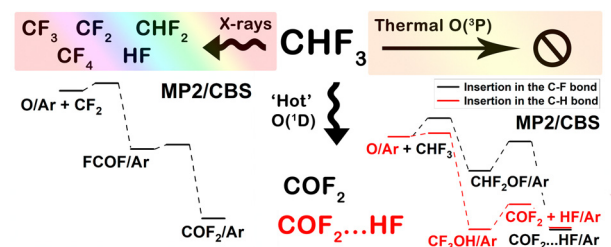
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Kang Jia, Xiao-Jing Dong, Sheng-Shi Li, Wei-Xiao Ji and Chang-Wen Zhang\*

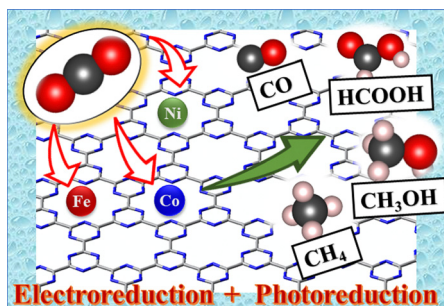
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Supriti Dutta and Swapan K. Pati\*

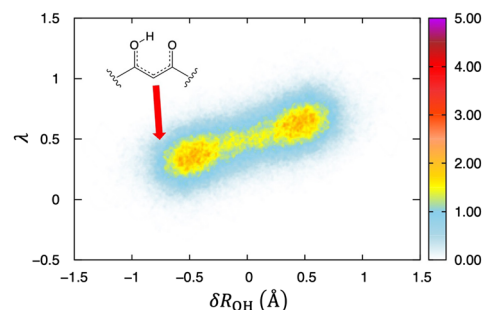


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**Nuclear quantum and H/D isotope effects on intramolecular hydrogen bond in curcumin**

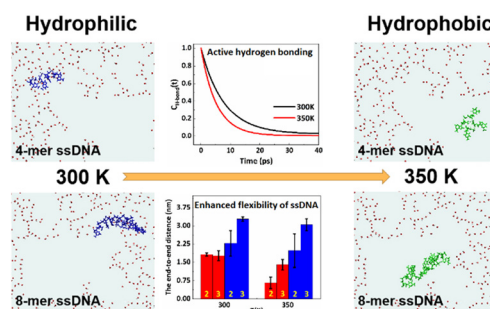
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**Dynamic behavior of the single-strand DNA molecules from the hydrophilic to hydrophobic regions on graphene oxide surface driven by heating**

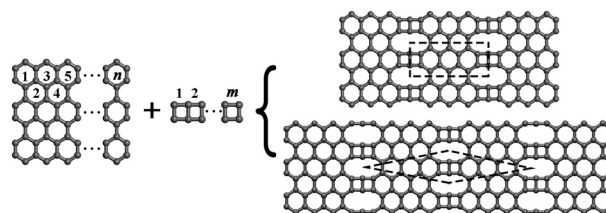
Mengjiao Wu, Yingying Huang, Li Yang, Yongshun Song\* and Xiaoling Lei\*



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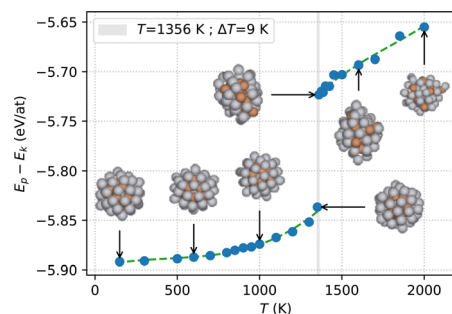
Guo Xiang Wang



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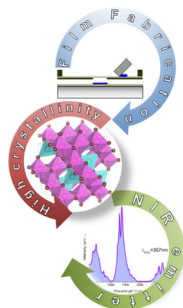
**Melting of FePt nanoparticles studied using DFT**

Paweł T. Jochym,\* Jan Łażewski and Przemysław Piekarczyk



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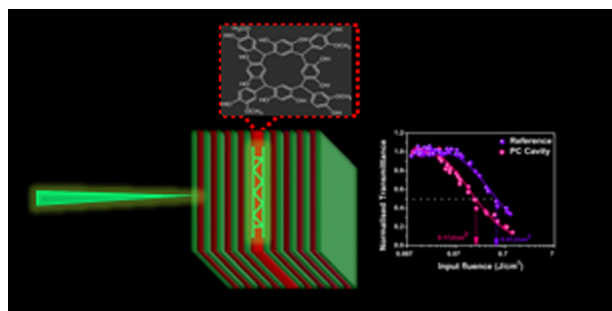
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### Cost-effective screen printing approach for Ce/Nd-doped $\text{ZnAl}_2\text{O}_4$ films: tuning crystallinity induced by the substrate

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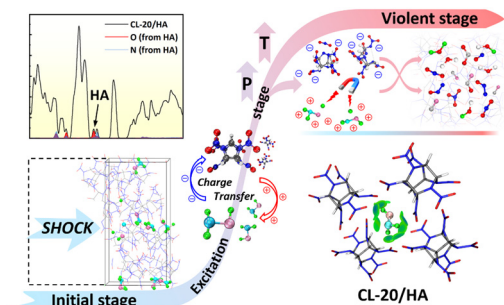
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Siji Alappattu John, Athulya Kadeprath Satheesan, Simi Pushpan K. and Chandrasekharan Keloth\*

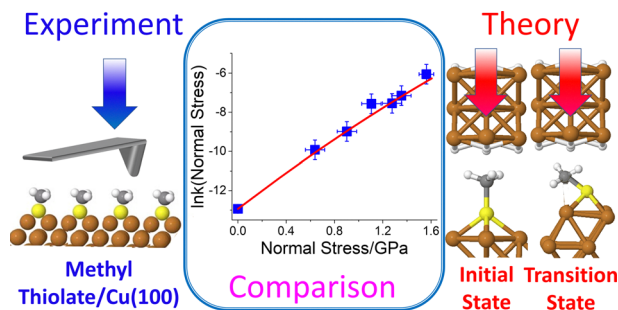
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Yiwen Xiao, Lang Chen,\* Kun Yang, Jianying Lu and Junying Wu

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



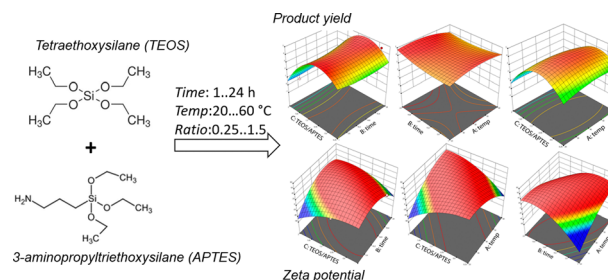


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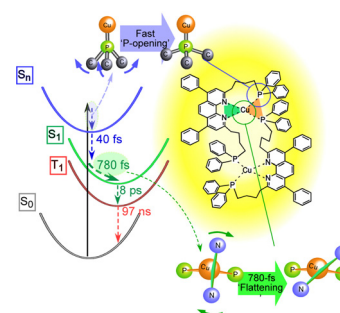
Lyubov Bondarenko,\* Yaroslav Saveliev, Dmitry Chernyaev, Rose Baimuratova, Gulzhian Dzhardimalieva, Artur Dzeranov, Elena Kelbysheva and Kamila Kydralieva



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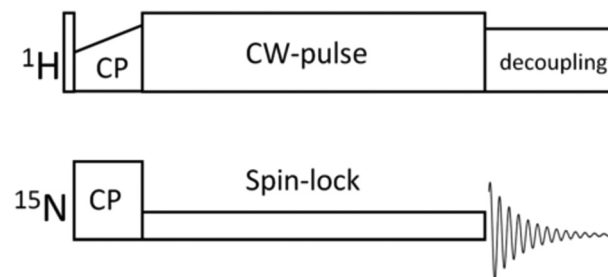
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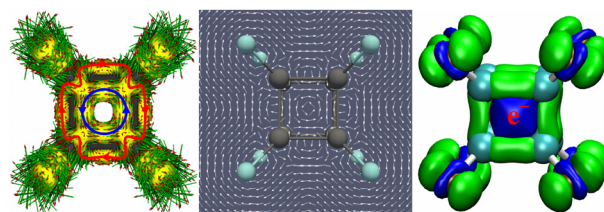
Alexey Krushelnitsky,\* Günter Hempel, Hannes Jurack and Tiago Mendes Ferreira



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

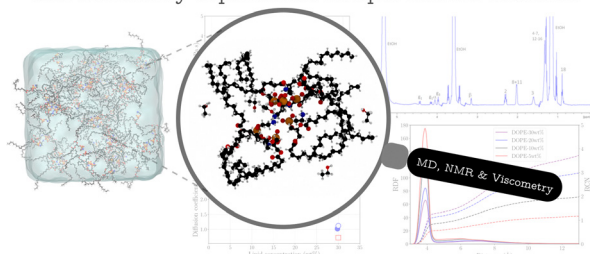
Xiaojun Li,\* Shuna Li, Jun Lu, Hongjiang Ren, Mengqi Zhang and Wangdi Zhang



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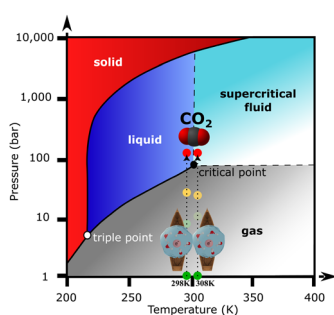
Simulation insight and interpretation of results from NMR and viscometry experiments in lipid-ethanol mixtures



### 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

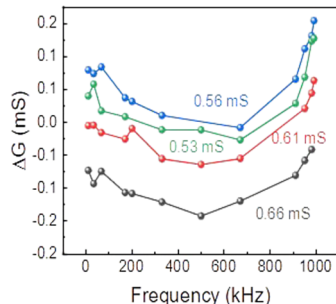
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### Reactivity of presolvated and solvated electrons with CO<sub>2</sub> in water up to 118 bar at 298 and 308 K

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Sergey A. Denisov\*

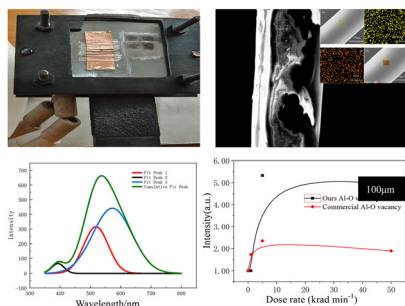
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### Tuning Bienenstock–Cooper–Munro learning rules in a two-terminal memristor for neuromorphic computing

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

Yang Shao, Yuting Wang\* and Xin Ju\*

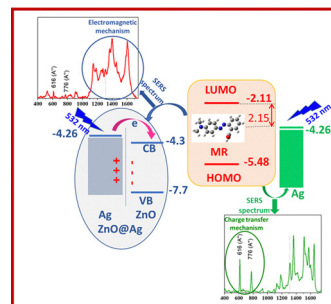


## RESEARCH PAPERS

15941

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

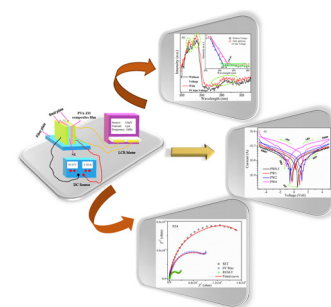
Thu Trang Tran, Xuan Hoa Vu, Thi Lan Ngo,  
Thi Thu Ha Pham,\* Dac Dien Nguyen and  
Van Dang Nguyen



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

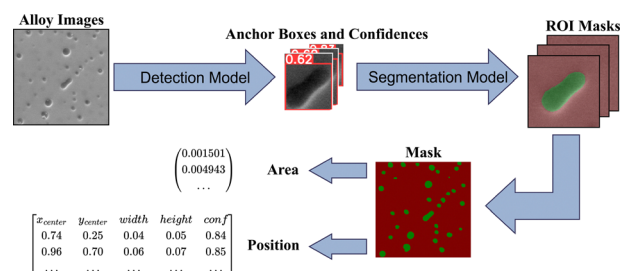
Riju Karmakar, Amit Kumar Das, Bilwadal Dutta,  
Subhojyoti Sinha,\* Saikat Santra, Subhamay Pramanik,  
Probodh Kumar Kuiri and Ajit Kumar Meikap\*



15970

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

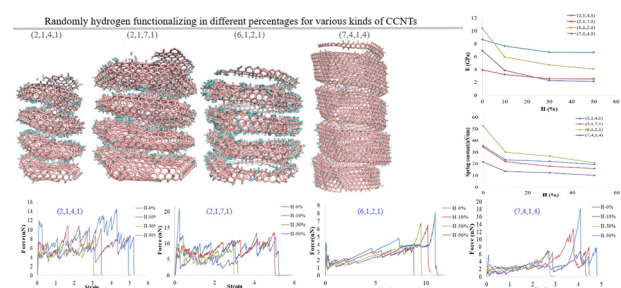
Zeyu Xia, Kan Ma, Sibo Cheng,\* Thomas Blackburn,  
Ziling Peng, Kewei Zhu, Weihang Zhang, Dunhui Xiao,  
Alexander J Knowles and Rossella Arcucci



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\*

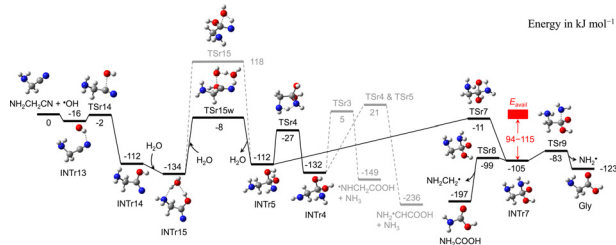


## RESEARCH PAPERS

16001

## Mechanisms of glycine formation from aminoacetonitrile in space

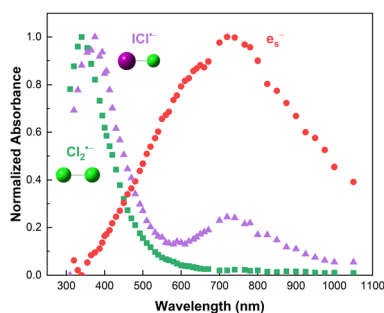
Joong Chul Choe



16009

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

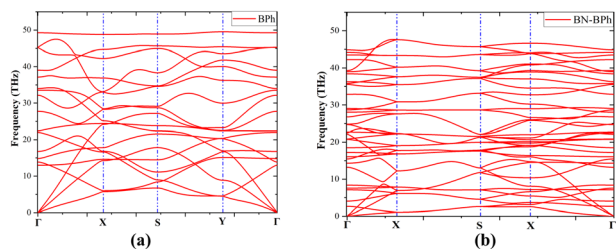
Jacy K. Conrad,\* Kazuhiro Iwamatsu, Michael E. Woods, Ruchi Gakhar, Bobby Layne, Andrew R. Cook and Gregory P. Horne\*



16018

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

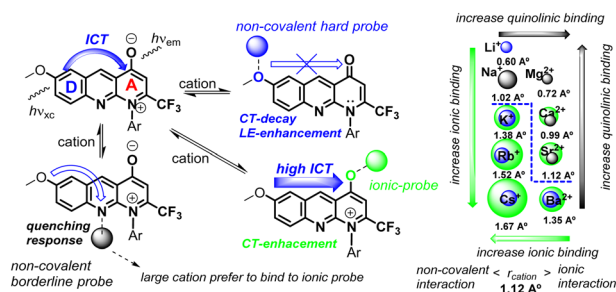
Mukesh Singh and Brahmananda Chakraborty\*



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

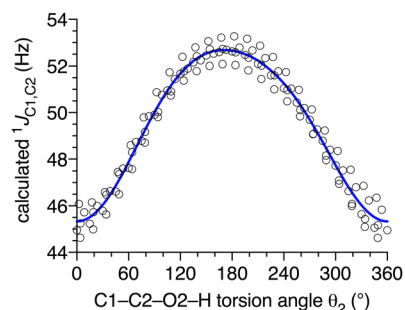


## RESEARCH PAPERS

16048

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

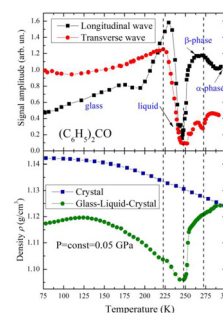
Timothy Tetrault, Reagan J. Meredith, Mi-Kyung Yoon, Christopher Canizares, Allen G. Oliver, Ian Carmichael and Anthony S. Serianni\*



16060

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

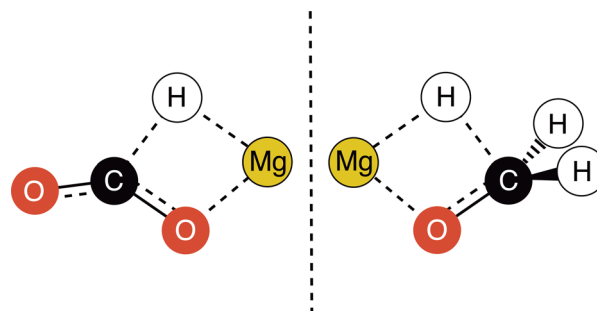
Elena L. Gromnitskaya,\* Igor V. Danilov, Fedor I. Zubkov and Vadim V. Brazhkin



16065

# Gas phase models of hydride transfer from divalent alkaline earth metals to $\text{CO}_2$ and $\text{CH}_2\text{O}$

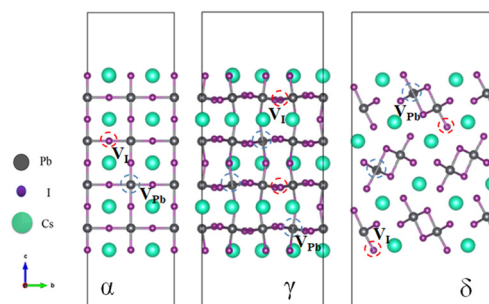
Christian Sant Gjermestad, Mauritz Johan Ryding and Einar Uggerud\*



16077

# Intrinsic defects on $\alpha$ , $\gamma$ and $\delta$ - $\text{CsPbI}_3$ (001) surfaces and implications for the $\alpha/\gamma$ to $\delta$ phase transition

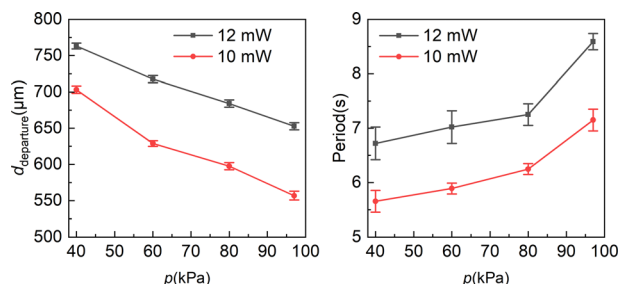
Na Wang\* and Yaqiong Wu





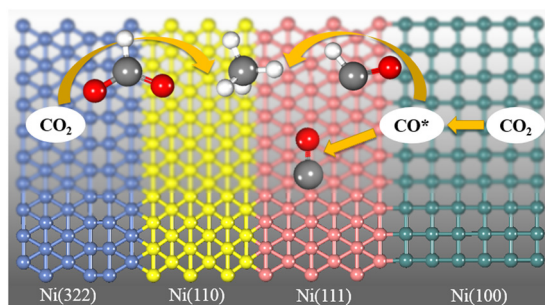
## RESEARCH PAPERS

16086

Influence of subatmospheric pressure on bubble evolution on the  $\text{TiO}_2$  photoelectrode surface

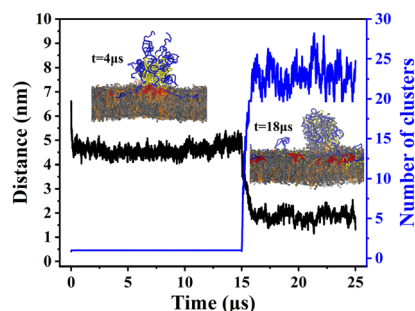
Xinyi Luo, Qiang Xu,\* Tengfei Nie, Yonglu She, Xingmiao Ye and Liejin Guo

16105

Mesoscale study of crystal-plane effects of Ni catalysts on  $\text{CO}_2$  hydrogenation

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

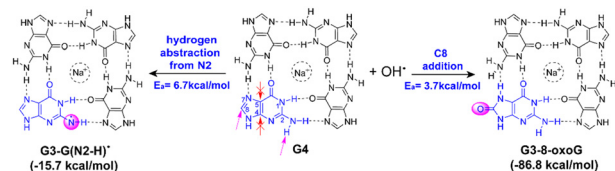
16114



## Delivery mechanism of doxorubicin by PEG-PPPE 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\*

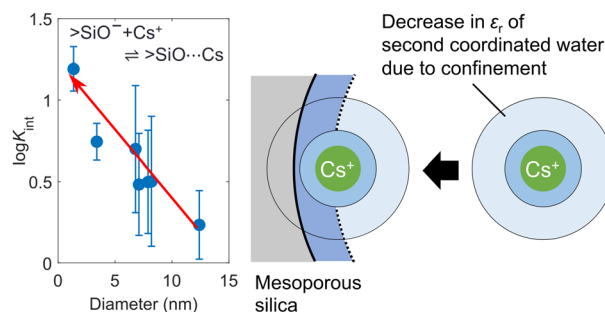


## RESEARCH PAPERS

16135

**Adsorption of cesium and strontium on mesoporous silicas**

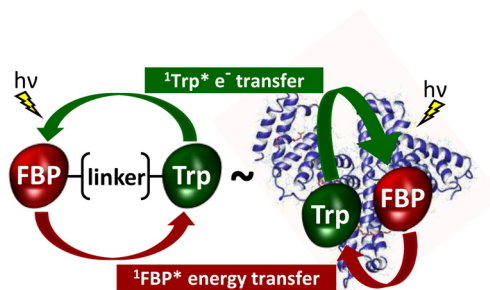
Kento Murota,\* Yoshio Takahashi and Takumi Saito



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

