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## IN THIS ISSUE

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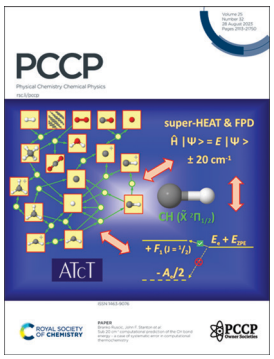


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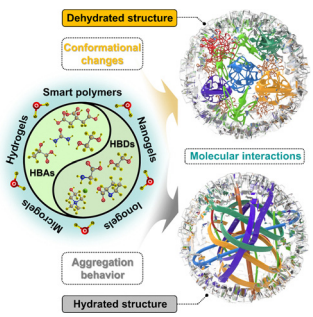


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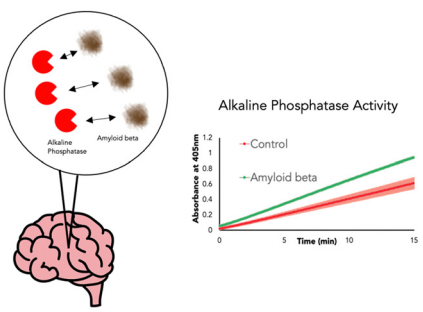

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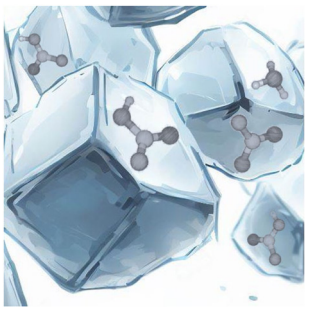



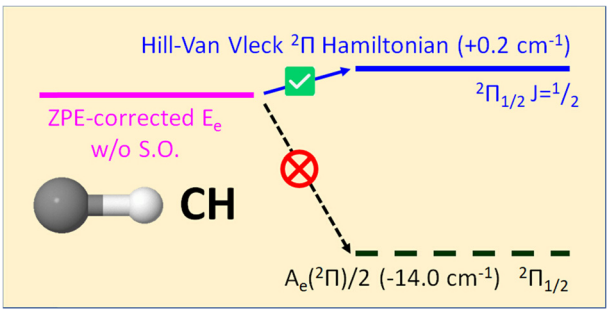




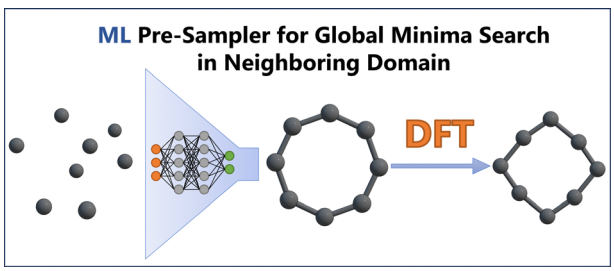




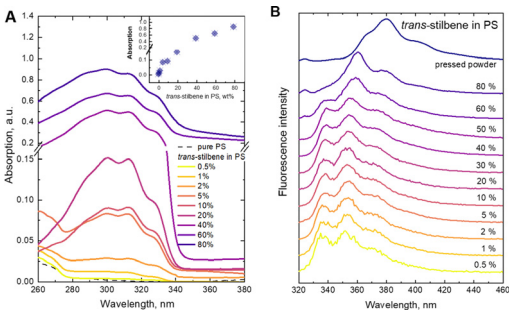

## RESEARCH PAPERS

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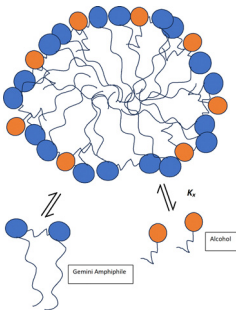
21236

## The partitioning of primary alcohols into the aggregates of gemini amphiphiles determined from diffusion NMR experiments

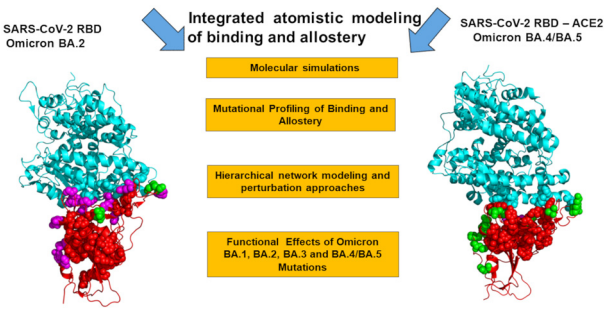
Brooke A. Morris, Ahmed A. Elgendy, Nicole E. MacNeil, Olivia M. Singer, Jacob G. Hoare, Robert D. Singer and D. Gerrard Marangoni*




21245

## Probing conformational landscapes of binding and allostery in the SARS-CoV-2 omicron variant complexes using microsecond atomistic simulations and perturbation-based profiling approaches: hidden role of omicron mutations as modulators of allosteric signaling and epistatic relationships

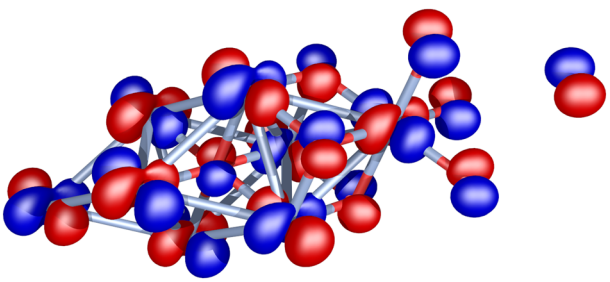
Gennady Verkhivker,* Mohammed Alshahrani, Grace Gupta, Sian Xiao and Peng Tao




21267

## Natural orbitals and two-particle correlators as tools for the analysis of effective exchange couplings in solids

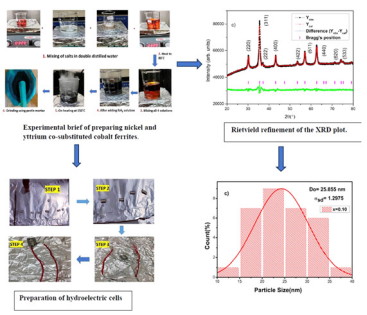
Pavel Pokhilko* and Dominika Zgid



21280

## Unveiling the impact of $Ni^{2+}/Y^{3+}$ co-substitution on the structural, dielectric, and impedance properties of multiferroic spinel ferrite for hydroelectric cell application

Prachi Jain, S. Shankar* and O. P. Thakur*



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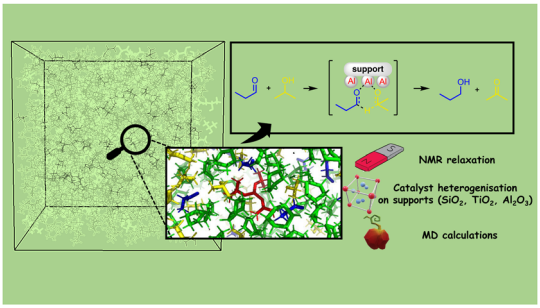




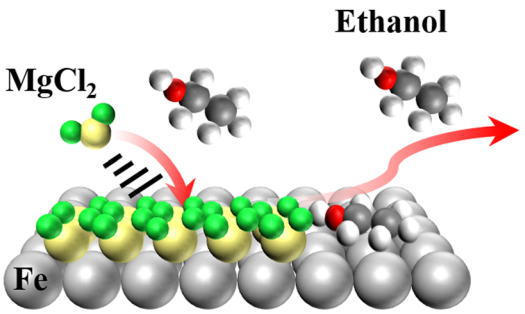




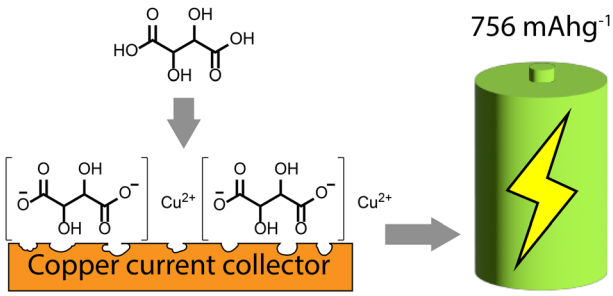




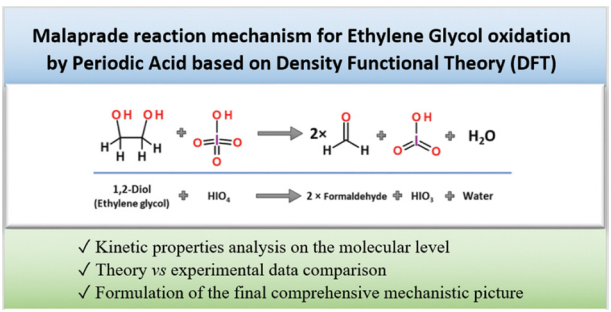

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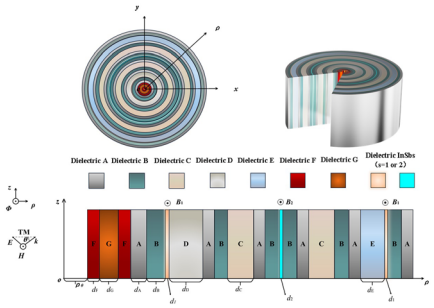
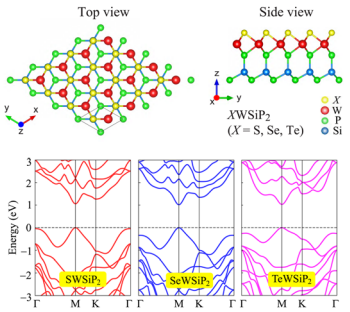
21456




## The multiple physical quantity sensor based on cylindrical photonic crystals with XOR logic gates

Ding-Yuan Zhang, Jun-Yang Sui, You-Ming Liu and Hai-Feng Zhang*

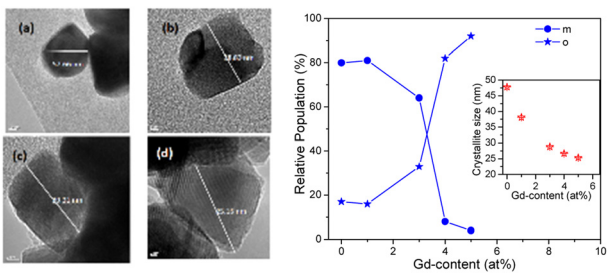
21468




## Moderate direct band-gap energies and high carrier mobilities of Janus $XWSiP_2$ (X = S, Se, Te) monolayers *via* first-principles investigation

Hiep T. Nguyen, Nguyen Q. Cuong, Vo T. T. Vi,* Nguyen N. Hieu and Linh P. T. Tran

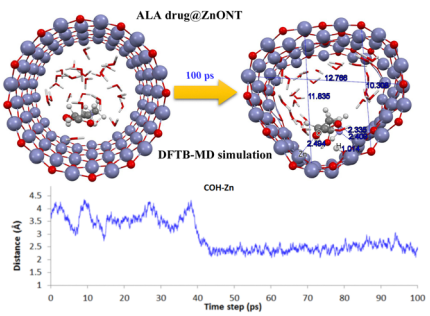
21479




## Comprehensive study on the origin of orthorhombic phase stabilization in Gd-doped $HfO_2$ and DFT calculations

D. Banerjee,* C. C. Dey, Ravi Kumar, Brindaban Modak, Snehamoyee Hazra, Subarna Datta, Barnali Ghosh, S. V. Thakare, S. N. Jha and D. Bhattacharyya

21492




## Toward functionalization of ZnO nanotubes and monolayers with 5-aminolevulinic acid drugs as possible nanocarriers for drug delivery: a DFT based molecular dynamic simulation

Masoumeh Mohammadzaheri, Saeed Jamehbozorgi,* Maosud Darvish Ganji, Mahyar Rezvani* and Zahra Javanshir

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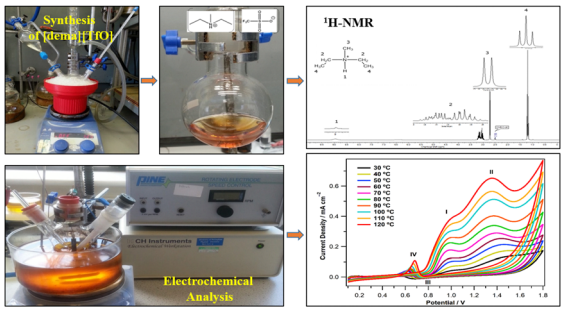




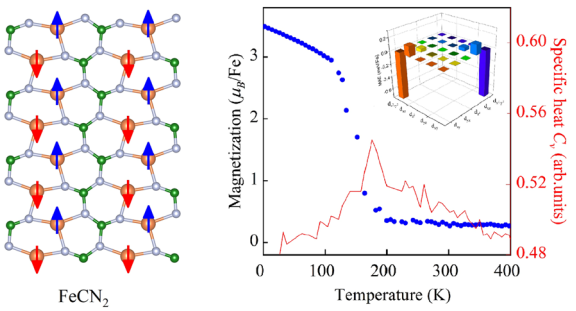




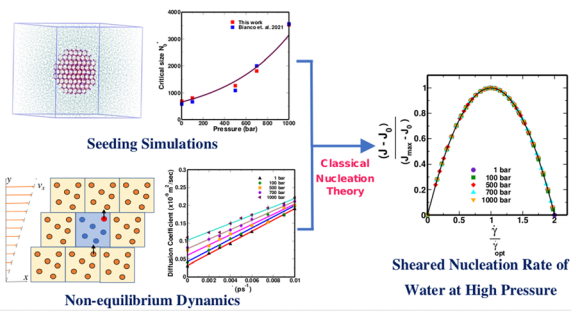




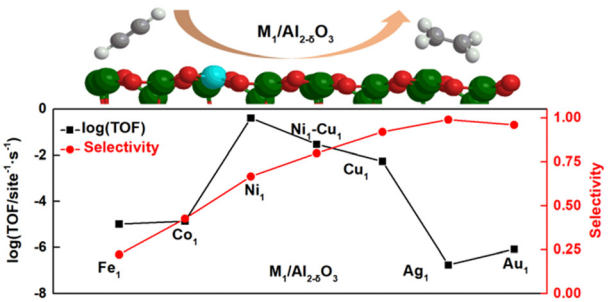

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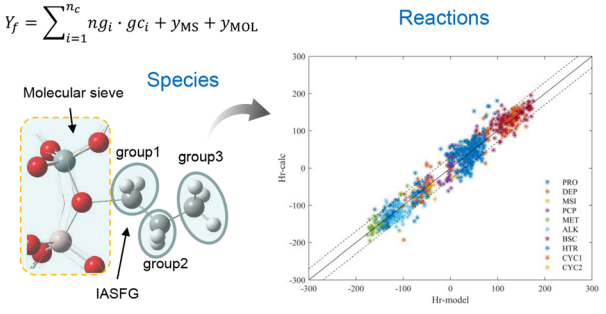
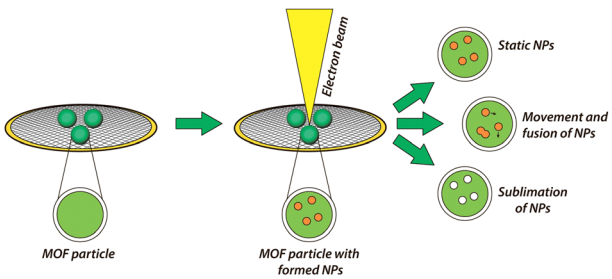
21631




### A modified group contribution method for estimating thermodynamic parameters of methanol-to-olefins over a SAPO-34 catalyst

Junyi Yu, Hua Li,* Mao Ye* and Zhongmin Liu

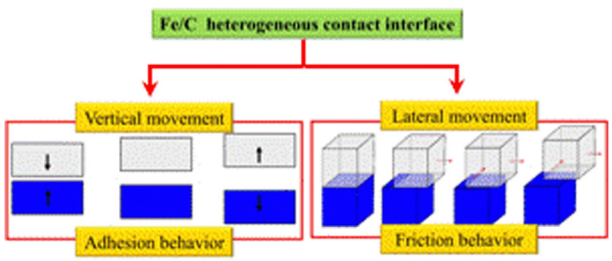
21640




### Dynamic behavior of metal nanoparticles in MOF materials: analysis with electron microscopy and deep learning

Kirill S. Erokhin, Evgeniy O. Pentsak, Vyacheslav R. Sorokin, Yury V. Agaev, Roman G. Zaytsev, Vera I. Isaeva and Valentine P. Ananikov*

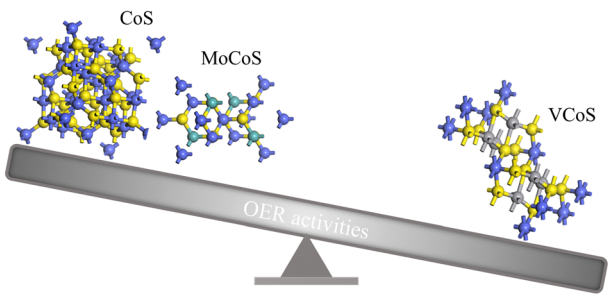
21649




### Adhesion and friction behaviors of a γ-Fe/diamond heterogeneous contact interface: a density functional theory study

Qizhen He, Lixiang Rao,* Wenwei Song, Hailiang Liu, Silong Zhang, Xuejun Ren and Qingxiang Yang*

21661




### Experimentally revealed and theoretically certified synergistic electronic interaction of V-doped CoS for facilitating the oxygen evolution reaction

Jingjing Zhang, Wei Deng,* Yun Weng, Xiang Li, Haifang Mao,* Tiandong Lu, Wenqian Zhang, Dewu Long and Fei Jiang*

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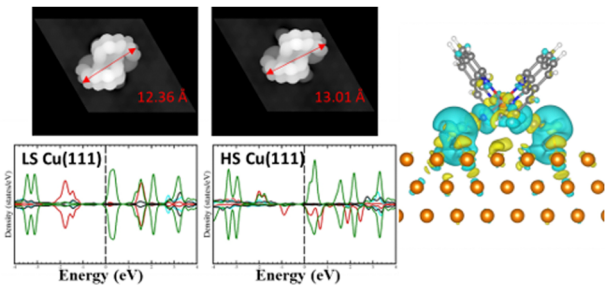
21673

## How complex–surface interactions modulate the spin transition of Fe(II) SCO complexes supported on metallic surfaces?

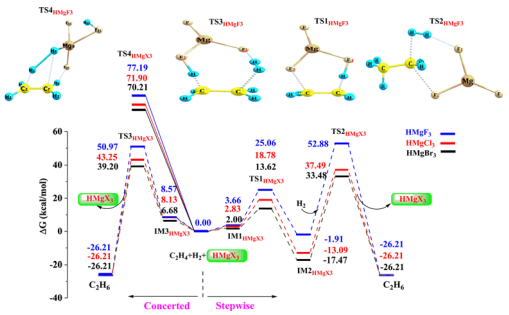
Rocío Sánchez-de-Armas,* Iman Jaber El lala and Carmen J. Calzado




21684

## Unveiling the correlation between the catalytic efficiency and acidity of a metal-free catalyst in a hydrogenation reaction. A theoretical case study of the hydrogenation of ethene catalyzed by a superacid arising from a superhalogen

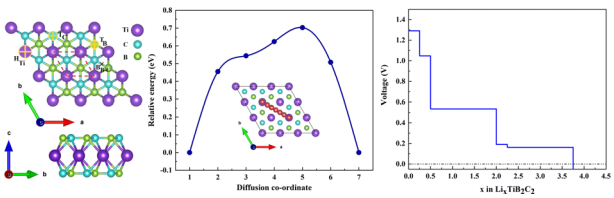
Jin-Feng Li,* Lan Luo, Zhi-Hui Bai and Bing Yin*




21699

## Two-dimensional Dirac $TiB_2C_2$ as a potential anode material for Li-ion batteries: a first-principles study

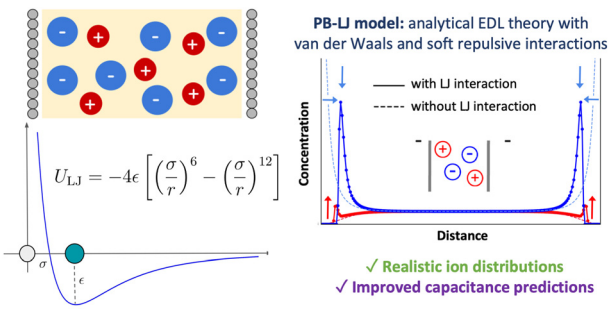
A. Etrini,* A. Elomrani, S. Oukahou, M. Maymoun, K. Sbiaai and A. Hasnaoui*




21708

## Incorporating ion-specific van der Waals and soft repulsive interactions in the Poisson–Boltzmann theory of electrical double layers

Aniruddha Seal, Utkarsh Tiwari, Ankur Gupta and Ananth Govind Rajan*



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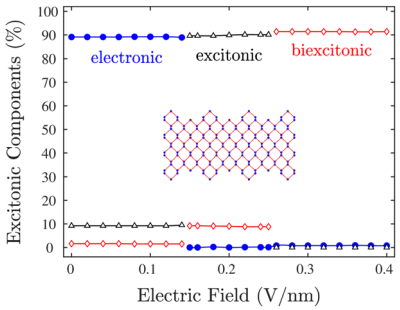
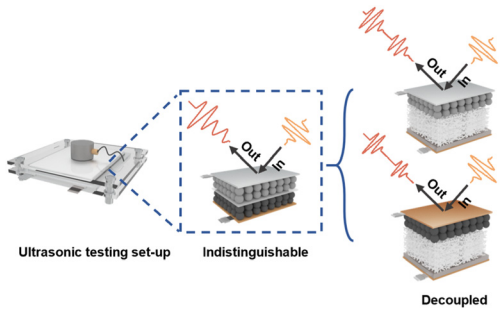



### Excitonic ground states in phosphorene nanoflakes

Jun Zhong, Wenzhuo Huang and Weidong Sheng*

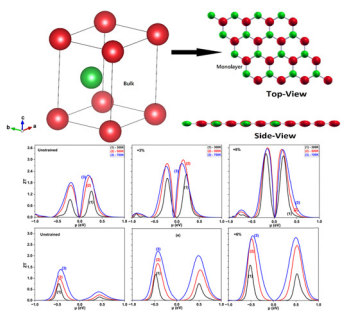
21730




### Decoupling of the anode and cathode ultrasonic responses to the state of charge of a lithium-ion battery

Xueting Liu, Zhe Deng, Yaqi Liao, Jinqiao Du, Jie Tian, Zijun Liu, Yue Shen* and Yunhui Huang*

21736




### Intrinsic and strain dependent ultralow thermal conductivity in novel AuX (X = Cu, Ag) monolayers for outstanding thermoelectric applications

Aadil Fayaz Wani, Shakeel Ahmad Khandy,* Lokanath Patra, Marutheeswaran Srinivasan, Jaspal Singh, Atif Mossad Ali, Ishtihadah Islam, Shobhna Dhiman and Kulwinder Kaur*