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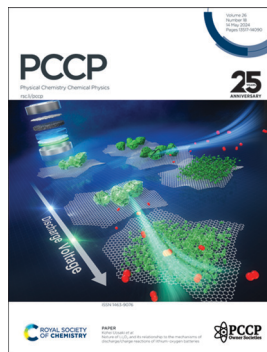
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ISSN 1463–9076 CODEN PPCPFQ 26(18) 13517–14090 (2024)



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See Angela Dellai, Giacomo Prampolini, Frédéric Castet *et al.*, pp. 13639–13654. Image reproduced by permission of Frédéric Castet from *Phys. Chem. Chem. Phys.*, 2024, 26, 13639.



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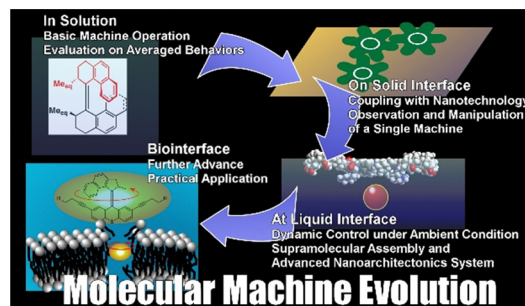
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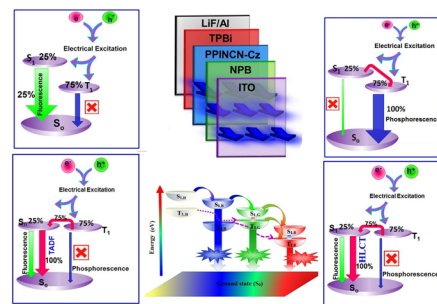
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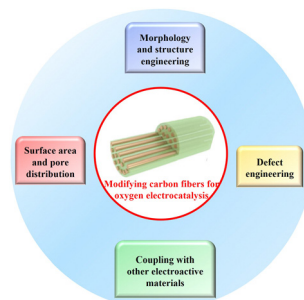


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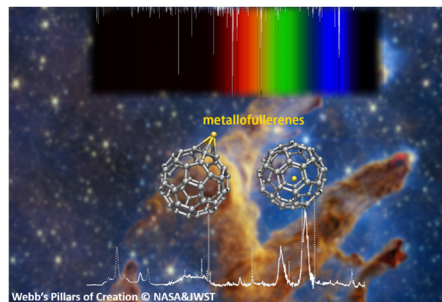


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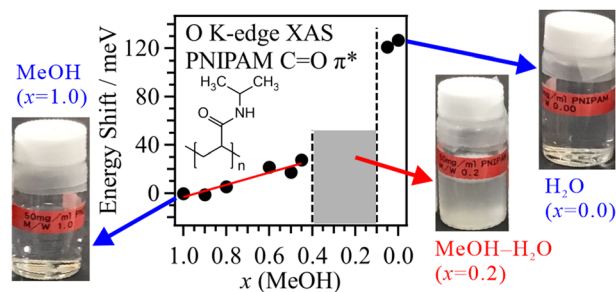


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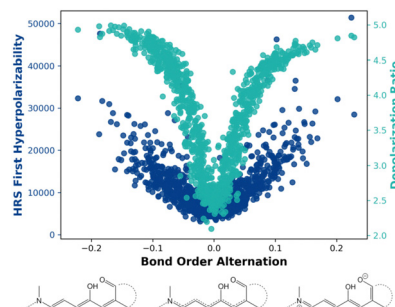


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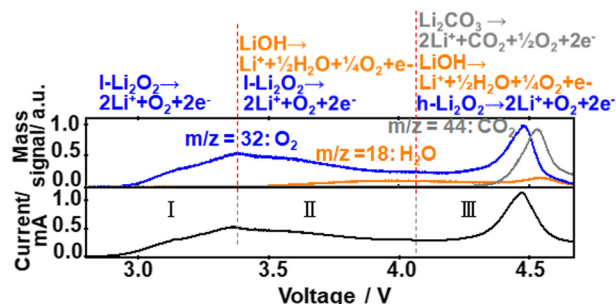
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## Dynamic effects on the nonlinear optical properties of donor acceptor stenhouse adducts: insights from combined MD + QM simulations

Angela Dellai,\* Carmelo Naim, Javier Cerezo, Giacomo Prampolini\* and Frédéric Castet\*



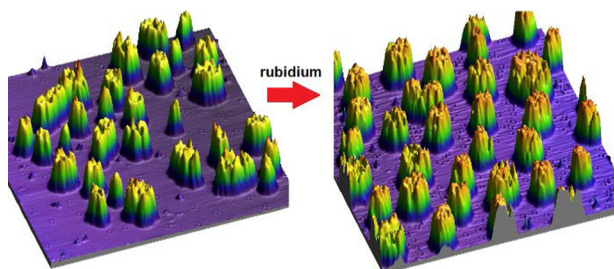
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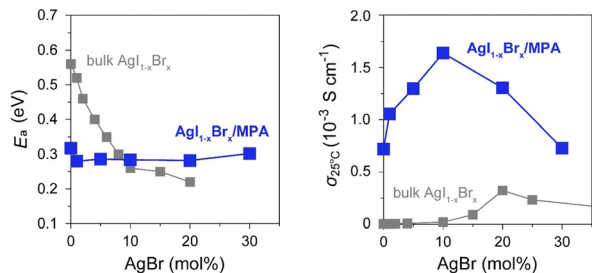


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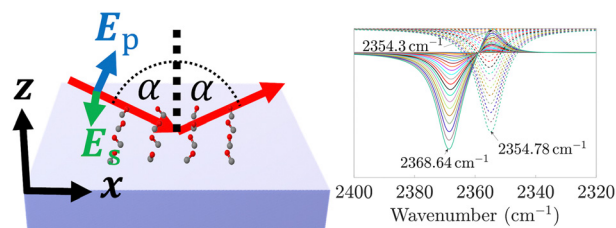
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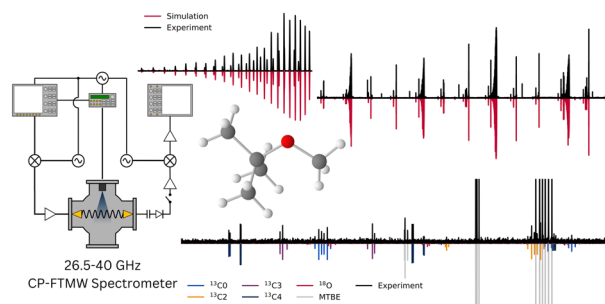


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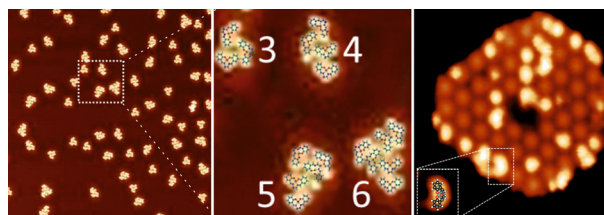
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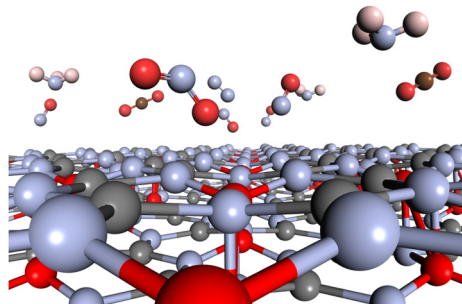
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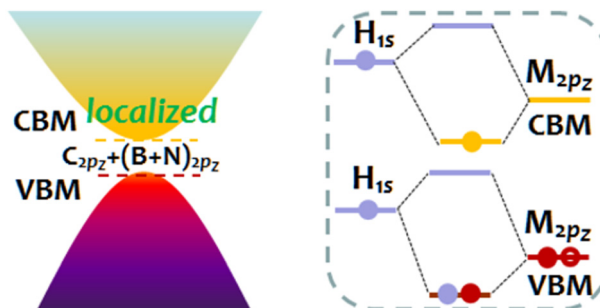
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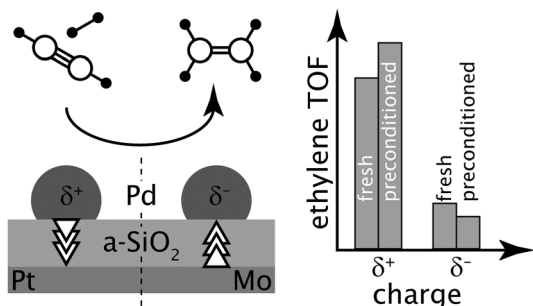
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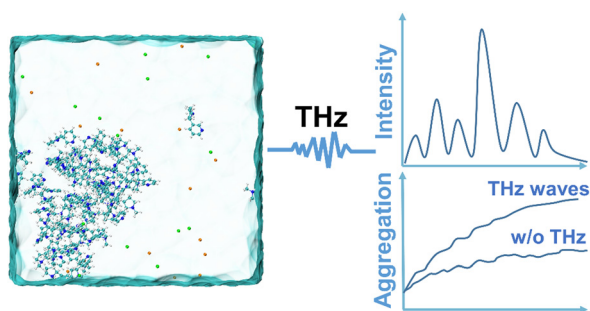
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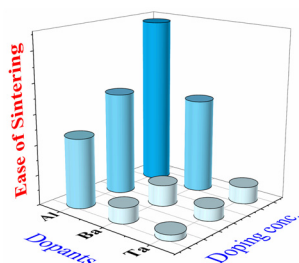
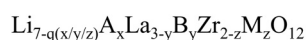
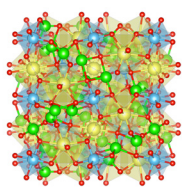
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### Effect of terahertz waves on the aggregation behavior of neurotransmitters

Meng-Qiu Li, Chen Chen, Yu-Qiang Ma and Hong-Ming Ding\*

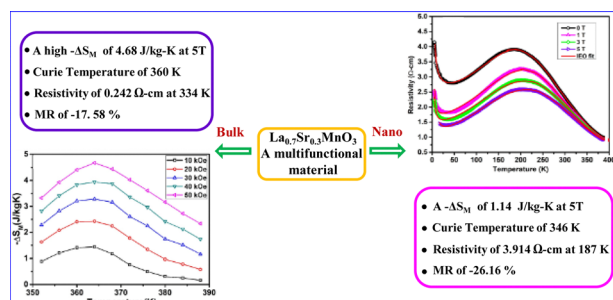
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Bhagya Uthaman,\* V. R. Akshay and Manoj Raama Varma

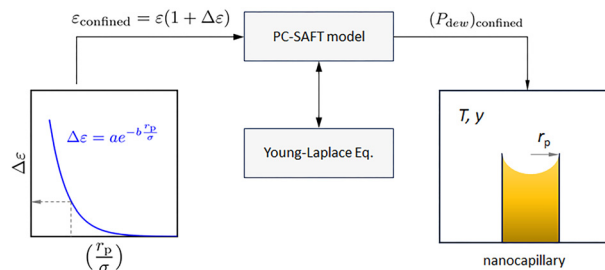


## RESEARCH PAPERS

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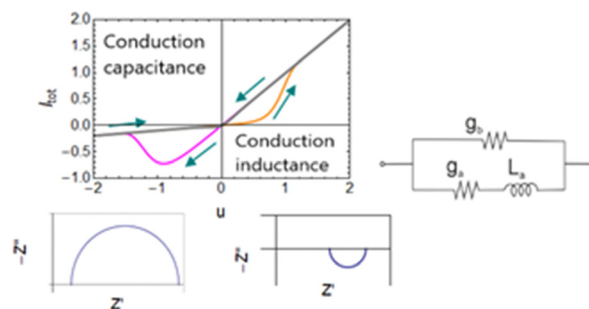
Aliakbar Roosta, Sohrab Zendeboudi and Nima Rezaei\*



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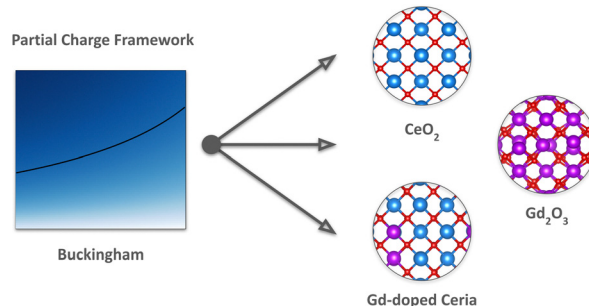
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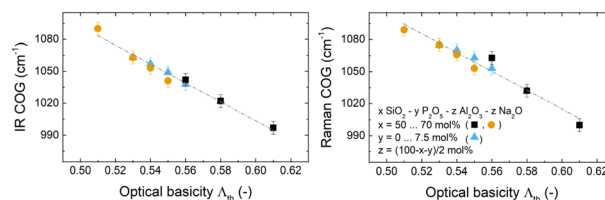
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## RESEARCH PAPERS

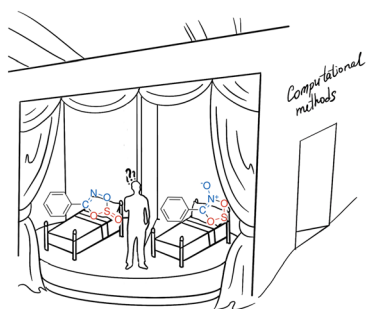
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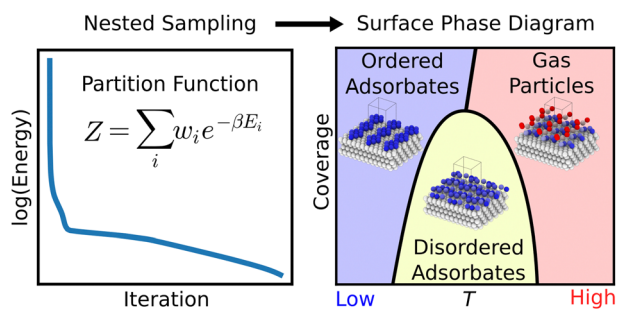
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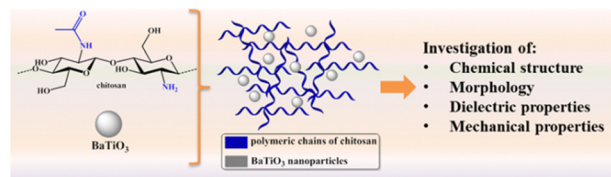
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### Surface phase diagrams from nested sampling

Mingrui Yang, Livia B. Pártay and Robert B. Wexler\*

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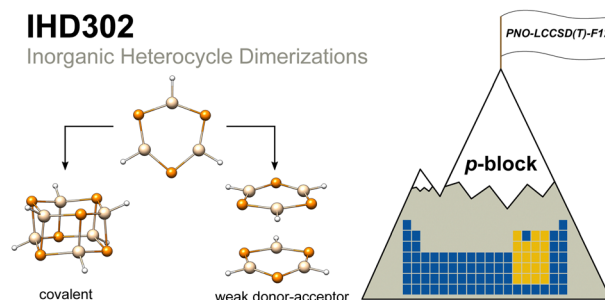
Razvan Rotaru, Violeta Melinte and Ioana-Sabina Trifan\*



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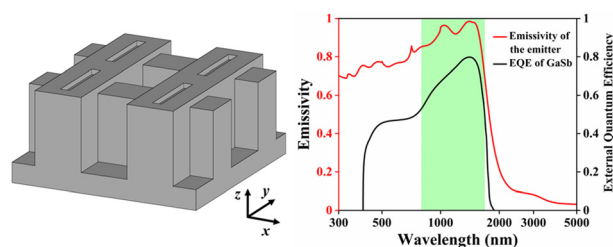
Thomas Gasevic, Markus Bursch,\* Qianli Ma, Stefan Grimme, Hans-Joachim Werner\* and Andreas Hansen\*



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### A tungsten-based metamaterial emitter for solar thermophotovoltaic systems

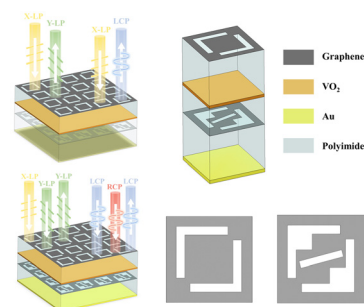
Yuchun Cao,\* Heng Zhang, Ning Chen, Haotuo Liu, Yongtao Feng and Xiaohu Wu\*



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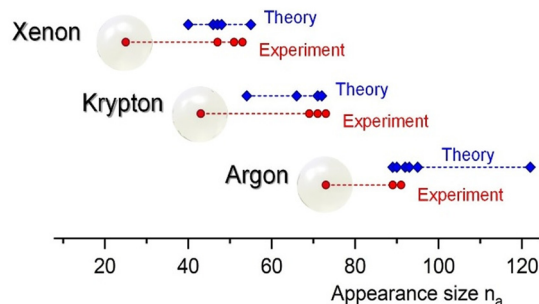
Xinzhi Zhang, Aihui Sun, Zhilong Jiang, Cheng Liu, Shouyu Wang and Yan Kong\*



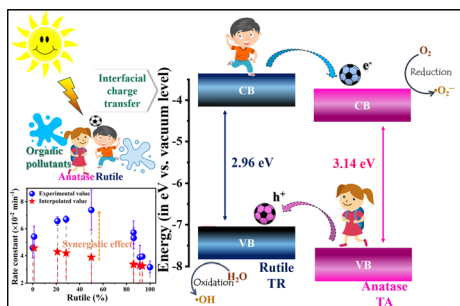
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### Size limits and fission channels of doubly charged noble gas clusters

Ianessa Stromberg, Stefan Bergmeister, Lisa Ganner, Fabio Zappa, Paul Scheier, Olof Echt\* and Elisabeth Gruber\*



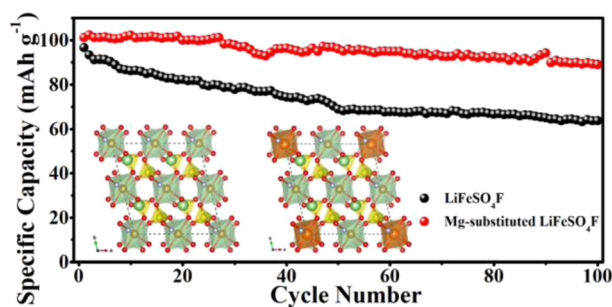
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Nimmy A. V., Anandakumar V. M. and Biju V.\*

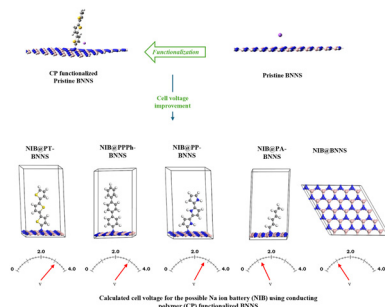
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### Improved structure stability and performance of a LiFeSO<sub>4</sub>F cathode material for lithium-ion batteries by magnesium substitution

Zhendong Guo, Tiejian Wang, Mingchen Ni, Fenhong Song, Jing Fan, Xiaorui Dong\* and Dashuai Wang\*

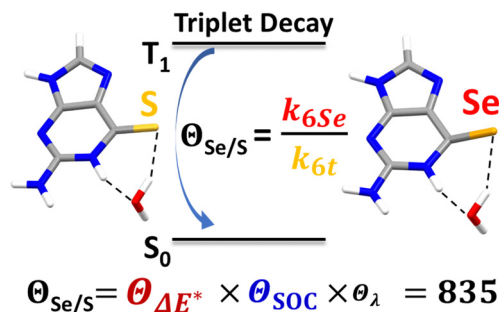
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### Anodic voltage performance of conducting polymer-functionalized boron nitride nanosheets: a DFT assessment

Chidera C. Nnadike, Hasnain Sajid, Ismail Abdulazeez and Abdulaziz A. Al-Saadi\*

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### Unexpected longer T<sub>1</sub> lifetime of 6-sulfur guanine than 6-selenium guanine: the solvent effect of hydrogen bonds to brake the triplet decay

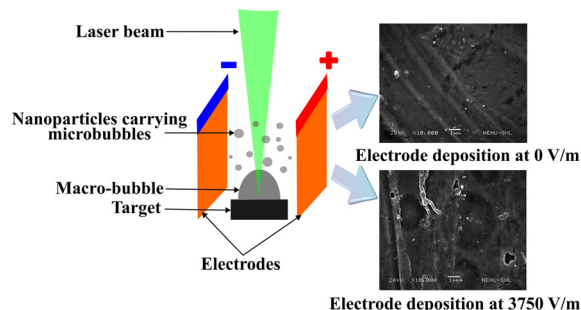
Shaoting Liu, Yuhuan Lee, Lingfang Chen, Jingheng Deng, Tongmei Ma,\* Mario Barbatti\* and Shuming Bai\*



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### Bubble-assisted microstreaming during electrode deposition of $\text{Mn}_2\text{O}_3$ energy harvesters

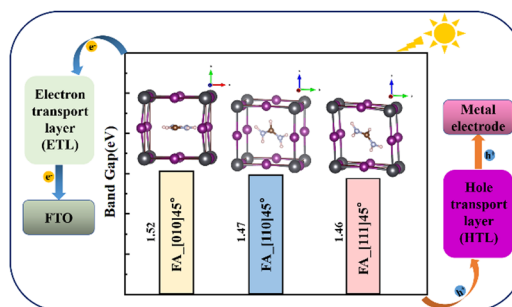
Sanchia Mae Kharphanbuh, Prahlad K. Baruah, Alika Khare and Arpita Nath\*



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### Regulating structural stability and photoelectrical properties of $\text{FAPbI}_3$ via formamidinium cation orientation

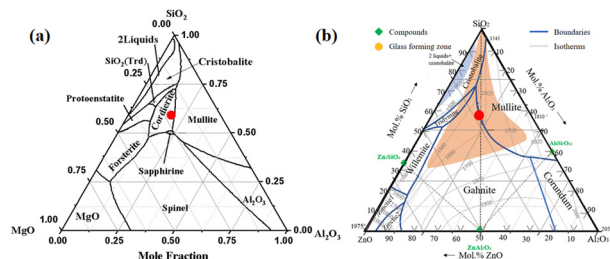
Shuning Wang, Qi Yang, Xiuchen Han, Dongmeng Chen, Bing Liu and Wenjing Fang\*



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### Impacts of substituting magnesium with zinc on crystallization behaviors in an aluminosilicate glass

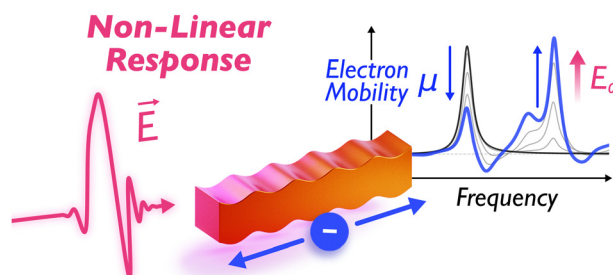
Biwei Huang, Qingshuang Zheng, Muzhi Cai, Ang Qiao and Haizheng Tao\*



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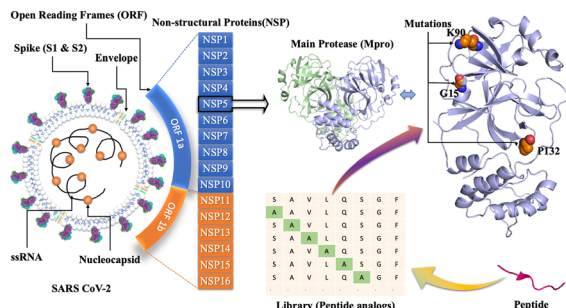
### Field-dependent THz transport nonlinearities in semiconductor nano structures

Quentin Wach, Michael T. Quick, Sabine Ayari and Alexander W. Achtstein\*



## RESEARCH PAPERS

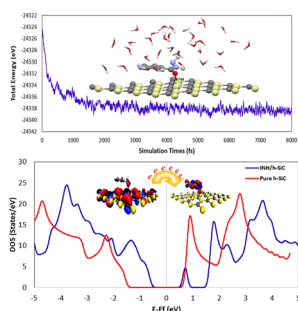
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### De novo design of potential peptide analogs against the main protease of Omicron variant using *in silico* studies

Stanly Paul M. L., Sonia Kumari, Tamás A. Martinek and Elizabeth Sobhia M.\*

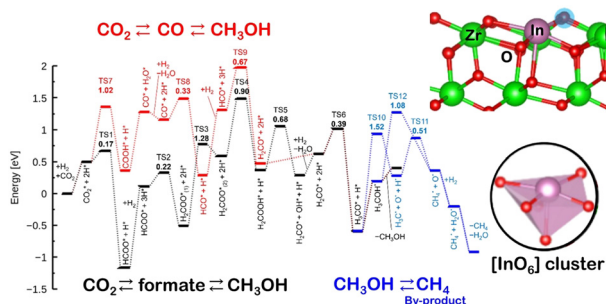
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### Unravelling performance of honeycomb structures as drug delivery systems for the izoniazid drug using DFT-D3 correction dispersion and molecular dynamic simulations

Masoud Darvish Ganji, Hyunseok Ko, Saeed Jamehbozorgi, Mahmood Tajbakhsh, Sepideh Tanreh, Rosa Pahlavan Nejad, Mahboubeh Sepahvand and Mahyar Rezvani\*

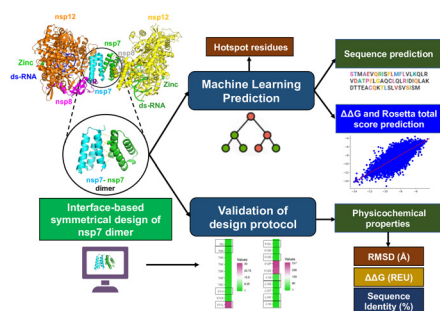
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### Difference in reaction mechanism between ZnZrO<sub>x</sub> and InZrO<sub>x</sub> for CO<sub>2</sub> hydrogenation

Shohei Tada,\* Yurika Ogura, Motohiro Sato, Akihiro Yoshida, Tetsuo Honma, Masahiko Nishijima, Tatsuya Joutsuka\* and Ryuji Kikuchi\*

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### Interface design of SARS-CoV-2 symmetrical nsp7 dimer and machine learning-guided nsp7 sequence prediction reveals physicochemical properties and hotspots for nsp7 stability, adaptation, and therapeutic design

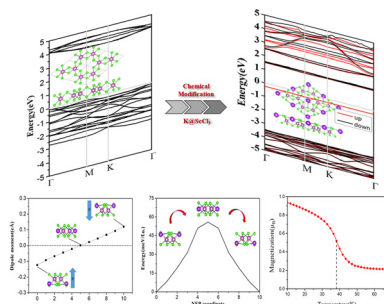
Amar Jeet Yadav, Shivank Kumar, Shweeta Maurya, Khushboo Bhagat and Aditya K. Padhi\*



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### Multiferroicity driven by single-atom adsorption on the two-dimensional semiconductor $\text{ScCl}_3$

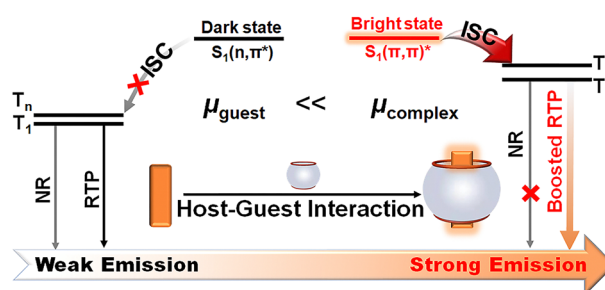
Yu Liang, Huasheng Sun, Xiang Li, Leichuang Zhu, Menghao Bi, Zhengxiao Du, Chengxi Huang\* and Fang Wu\*



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### Host-guest interaction induced room-temperature phosphorescence enhancement of organic dyes: a computational study

Xiaoli Luo, Yi Zeng, Haoran Wei and Xiaoyan Zheng\*



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### The oxygen evolution reaction on cobalt atom embedded nitrogen doped graphene electrocatalysts: a density functional theory study

Meijing Liao, Bing Zhao, Guangsong Zhang, Junhao Peng, Yuxing Zhang,\* Bin Liu\* and Xinfang Wang\*

