

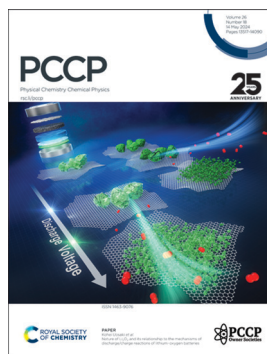
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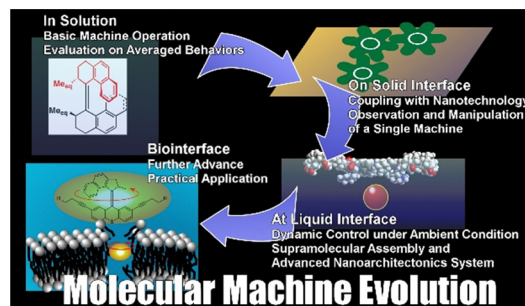
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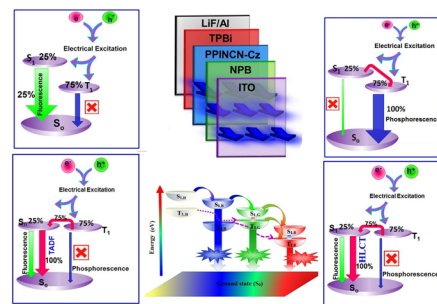
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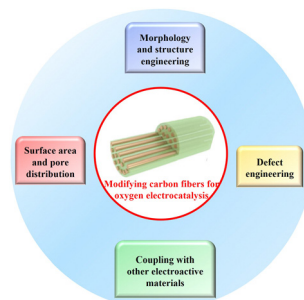


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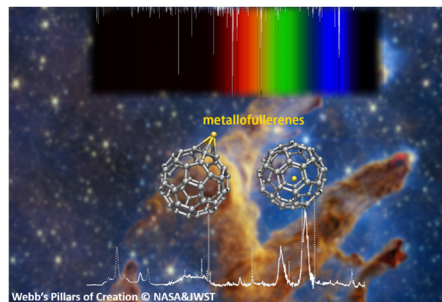


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Ransel Barzaga* and Gao-Lei Hou*

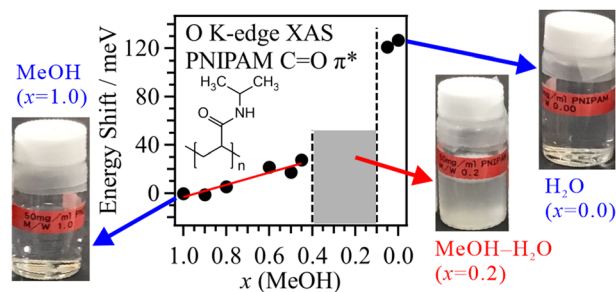


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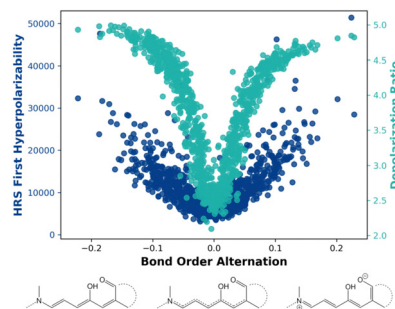


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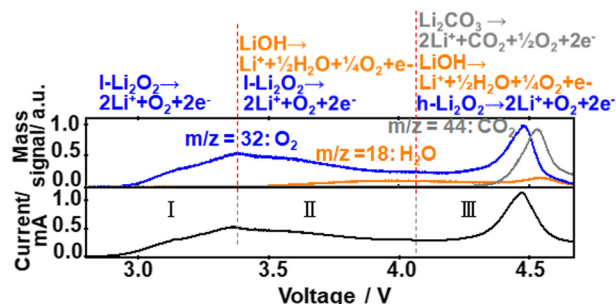
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Dynamic effects on the nonlinear optical properties of donor acceptor stenhouse adducts: insights from combined MD + QM simulations

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



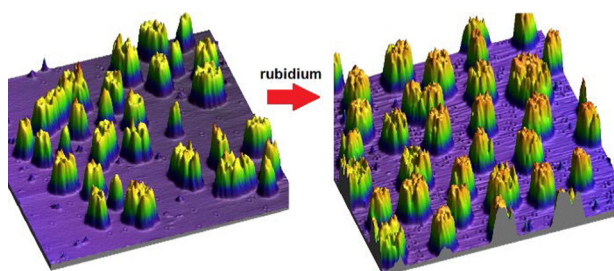
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Nature of Li_2O_2 and its relationship to the mechanisms of discharge/charge reactions of lithium–oxygen batteries

Yanan Gao, Hitoshi Asahina, Shoichi Matsuda, Hidenori Noguchi and Kohei Uosaki*

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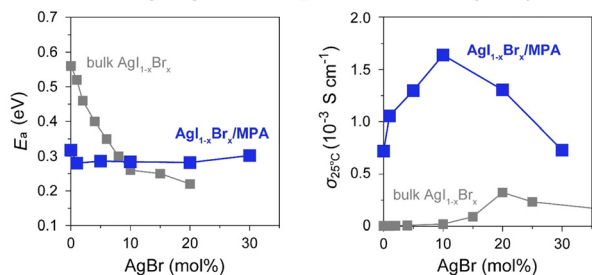


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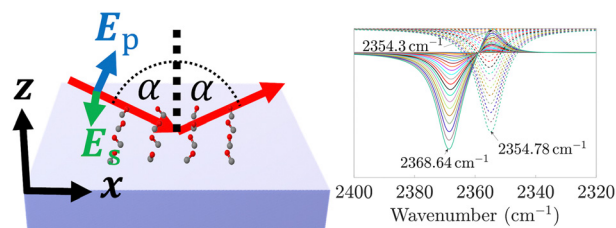
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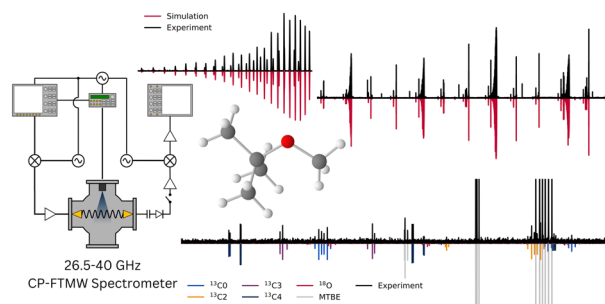


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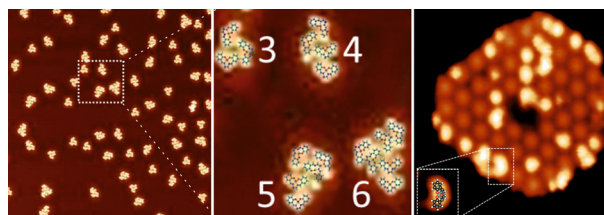
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An approach for patterned molecular adsorption on ferromagnets, achieved *via* Moiré superstructures

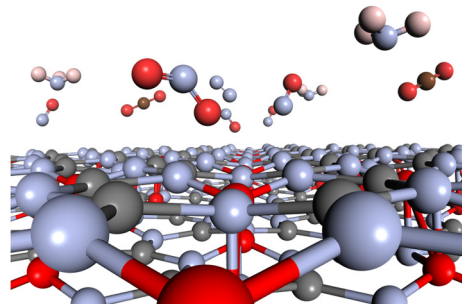
Sigmund Jensen, Isaac Appelquist Løge, Jesper Bendix and Lars Diekhöner*



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Atomic insights into the interaction of N_2 , CO_2 , NH_3 , NO , and NO_2 gas molecules with $Zn_2(V, Nb, Ta)N_3$ ternary nitride monolayers

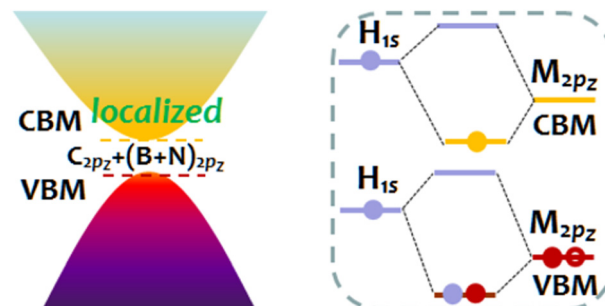
Andrey A. Kistanov



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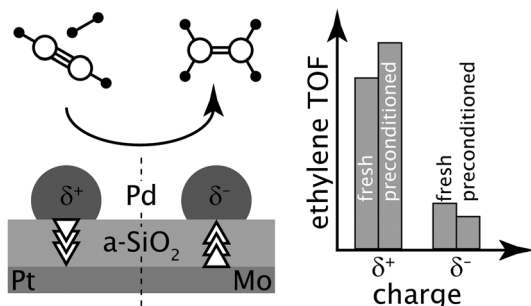
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Zhengyan Chen, Sanjun Wang, Wen Xiong and Fei Wang*



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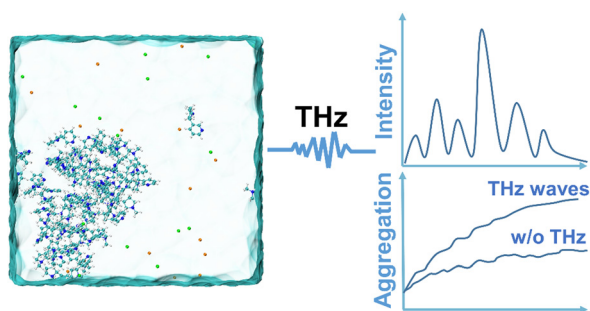
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Same size, same support, same spectator? Selective acetylene hydrogenation on supported Pd nanoparticles

Marian D. Rötzer, Maximilian Krause, Tobias Hinke, Kevin Bertrang, Florian F. Schweinberger, Andrew S. Crampton and Ueli Heiz*

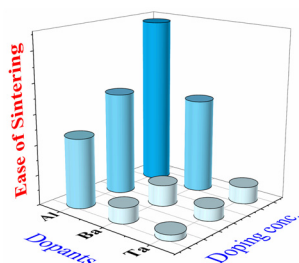
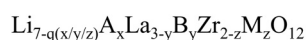
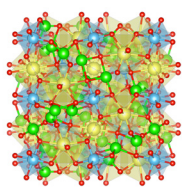
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Effect of terahertz waves on the aggregation behavior of neurotransmitters

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

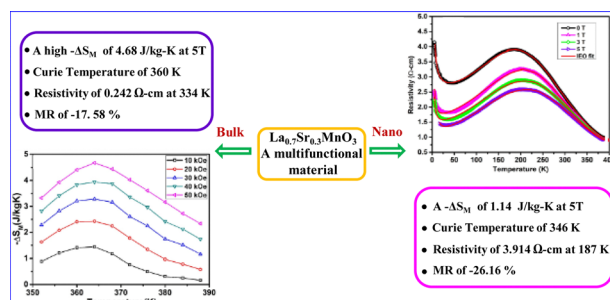
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First-principles evaluation of dopant impact on structural deformability and processability of $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$

A. Dive,* K. Kim, S. Kang, L. F. Wan* and B. C. Wood*

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

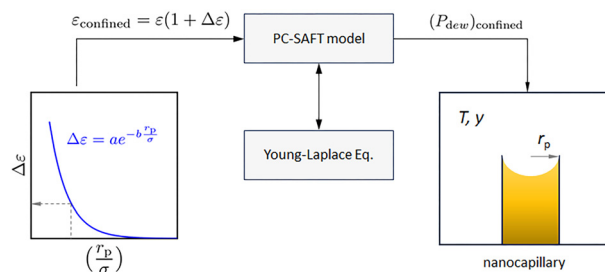


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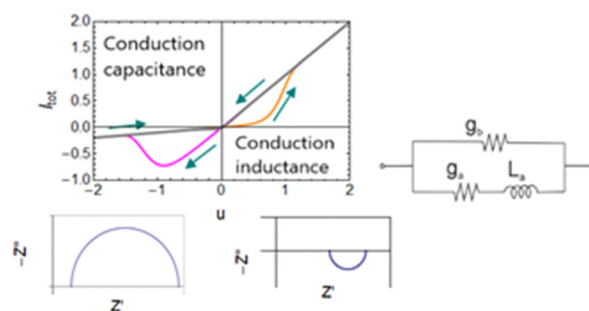
Aliakbar Roosta, Sohrab Zendehboudi and Nima Rezaei*



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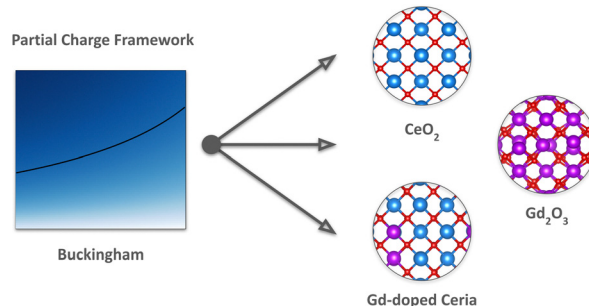
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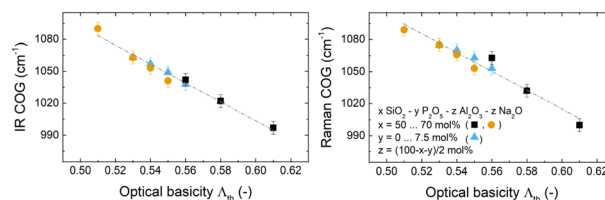
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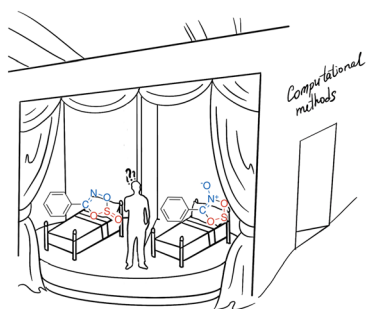
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Thermal properties of novel phase change materials based on protic ionic liquids containing ethanolamines and stearic acid for efficient thermal energy storage

Masumeh Mokhtarpour, Ali Rostami,* Hemayat Shekaari, Armin Zarghami and Saeid Faraji

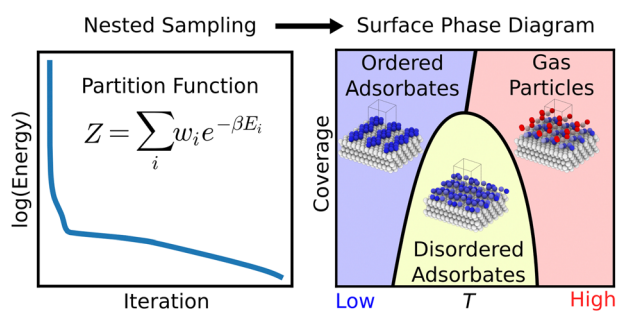
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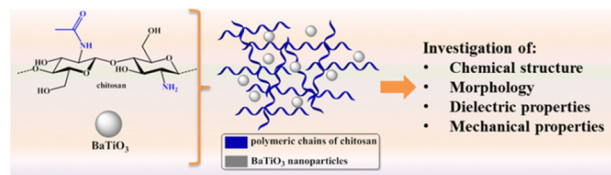
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Surface phase diagrams from nested sampling

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

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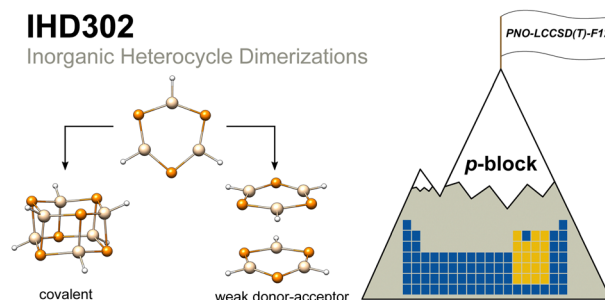
Razvan Rotaru, Violeta Melinte and Ioana-Sabina Trifan*



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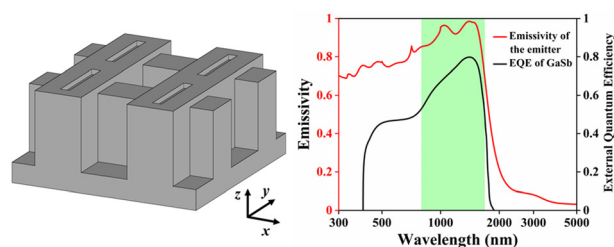
Thomas Gasevic, Markus Bursch,* Qianli Ma, Stefan Grimme, Hans-Joachim Werner* and Andreas Hansen*



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A tungsten-based metamaterial emitter for solar thermophotovoltaic systems

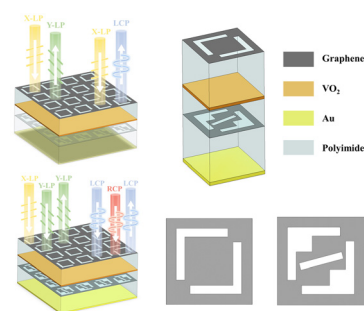
Yuchun Cao,* Heng Zhang, Ning Chen, Haotuo Liu, Yongtao Feng and Xiaohu Wu*



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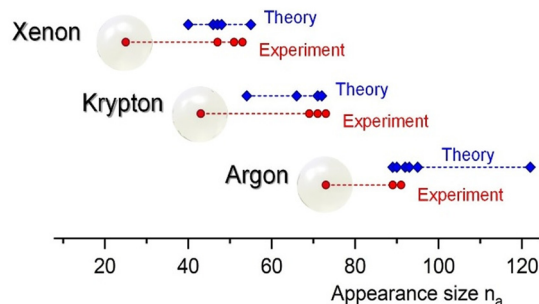
Xinzhi Zhang, Aihui Sun, Zhilong Jiang, Cheng Liu, Shouyu Wang and Yan Kong*



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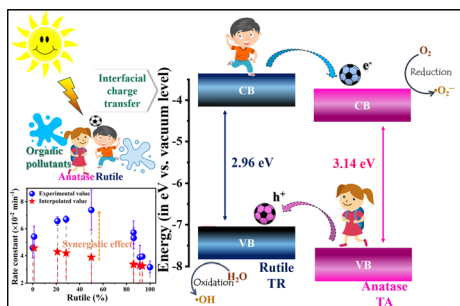
Size limits and fission channels of doubly charged noble gas clusters

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



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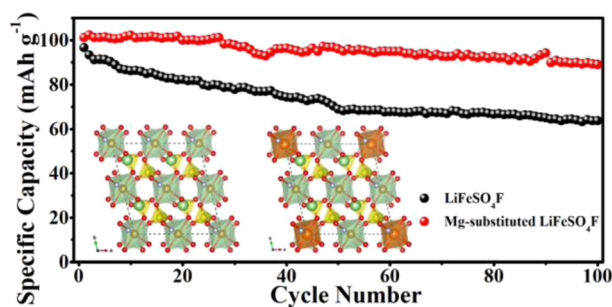
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Band alignment and interfacial charge transfer in sol-gel derived anatase/rutile heterophase TiO₂: explaining the synergistic photocatalytic activity

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

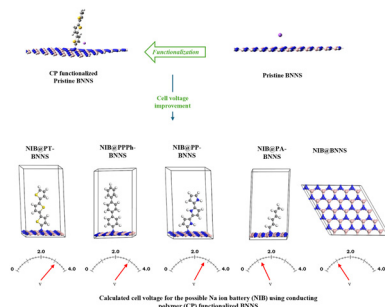
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Improved structure stability and performance of a LiFeSO₄F cathode material for lithium-ion batteries by magnesium substitution

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

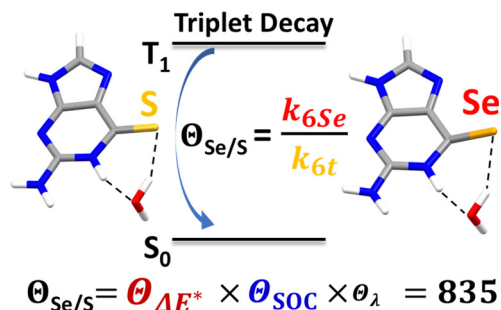
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Anodic voltage performance of conducting polymer-functionalized boron nitride nanosheets: a DFT assessment

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

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Unexpected longer T₁ lifetime of 6-sulfur guanine than 6-selenium guanine: the solvent effect of hydrogen bonds to brake the triplet decay

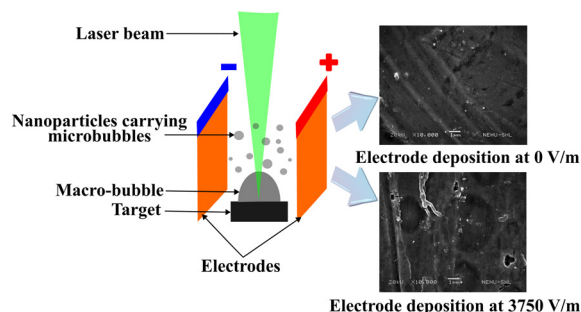
Shaoting Liu, Yuhuan Lee, Lingfang Chen, Jingheng Deng, Tongmei Ma,* Mario Barbatti* and Shuming Bai*



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Bubble-assisted microstreaming during electrode deposition of Mn_2O_3 energy harvesters

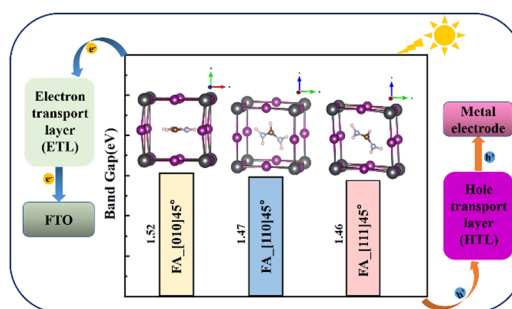
Sanchia Mae Kharphanbuh, Prahlad K. Baruah, Alika Khare and Arpita Nath*



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Regulating structural stability and photoelectrical properties of $FAPbI_3$ via formamidinium cation orientation

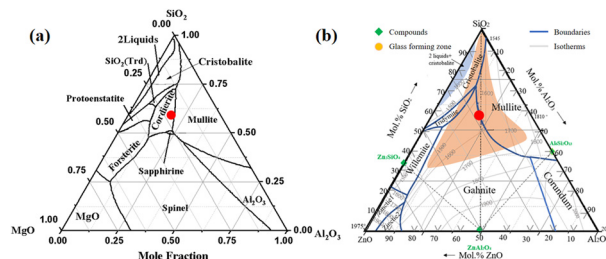
Shuning Wang, Qi Yang, Xiuchen Han, Dongmeng Chen, Bing Liu and Wenjing Fang*



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

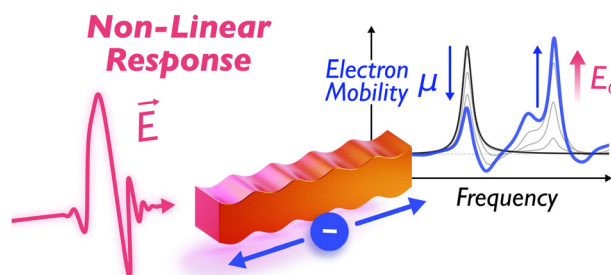
Biwei Huang, Qingshuang Zheng, Muzhi Cai, Ang Qiao and Haizheng Tao*



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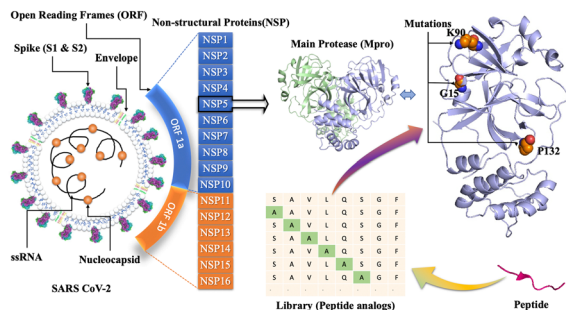
Field-dependent THz transport nonlinearities in semiconductor nano structures

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



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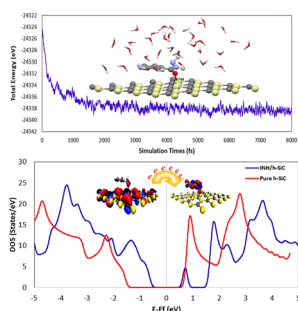
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De novo design of potential peptide analogs against the main protease of Omicron variant using *in silico* studies

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

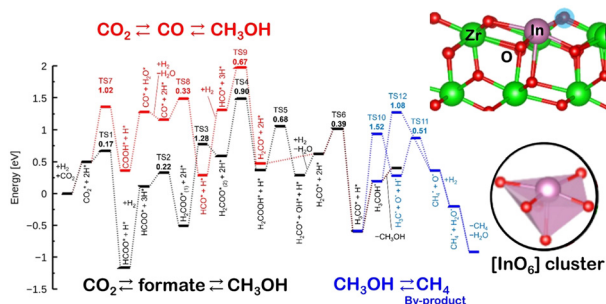
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Unravelling performance of honeycomb structures as drug delivery systems for the izoniazid drug using DFT-D3 correction dispersion and molecular dynamic simulations

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

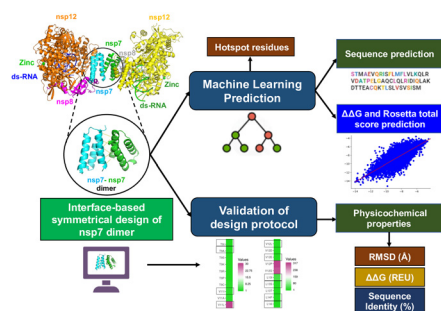
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Difference in reaction mechanism between ZnZrO_x and InZrO_x for CO₂ hydrogenation

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

14046



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

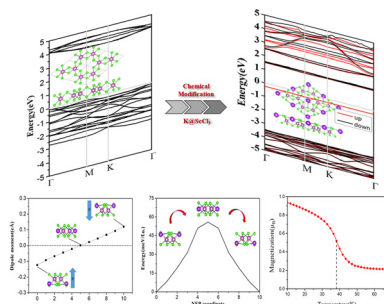
Amar Jeet Yadav, Shivank Kumar, Shweeta Maurya, Khushboo Bhagat and Aditya K. Padhi*



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Multiferroicity driven by single-atom adsorption on the two-dimensional semiconductor ScCl_3

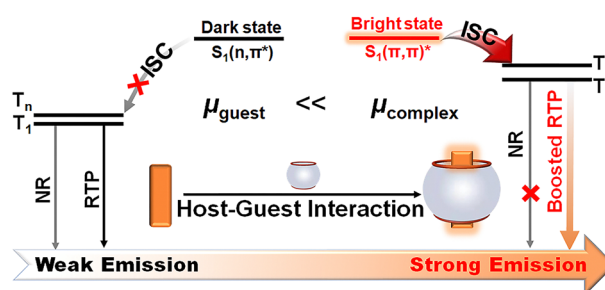
Yu Liang, Huasheng Sun, Xiang Li, Leichuang Zhu, Menghao Bi, Zhengxiao Du, Chengxi Huang* and Fang Wu*



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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*

