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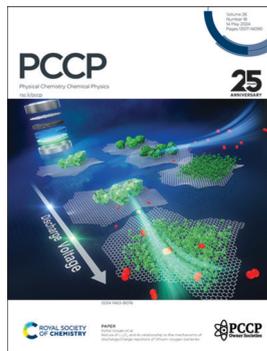
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ISSN 1463–9076 CODEN PPCPFQ 26(18) 13517–14090 (2024)



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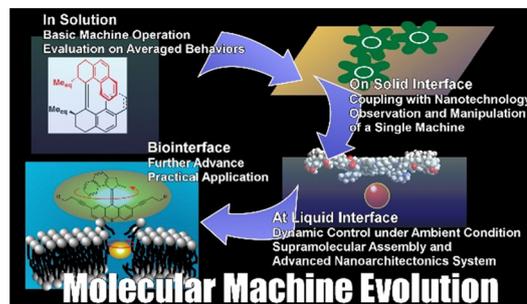
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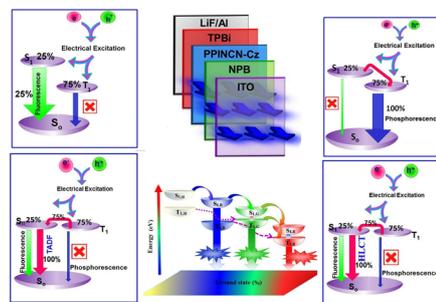
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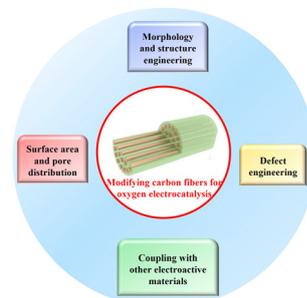


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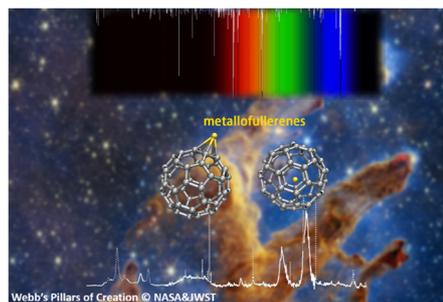


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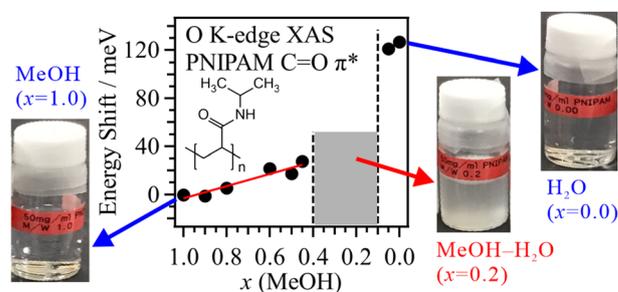


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Masanari Nagasaka,* Fumitoshi Kumaki, Yifeng Yao, Jun-ichi Adachi and Kenji Mochizuki

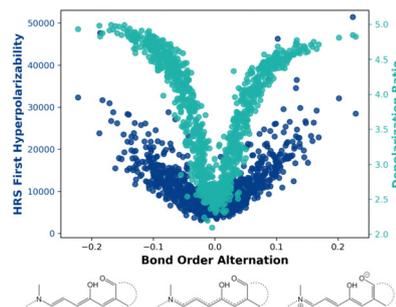


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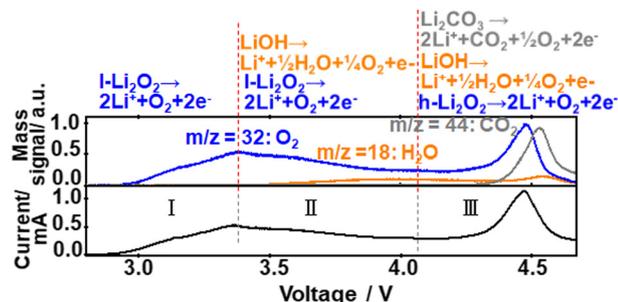
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Dynamic effects on the nonlinear optical properties of donor acceptor stenhouse adducts: insights from combined MD + QM simulations

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



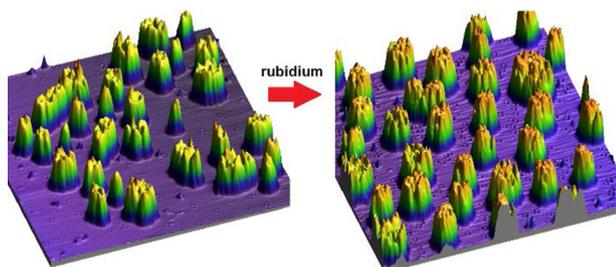
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Yanan Gao, Hitoshi Asahina, Shoichi Matsuda, Hidenori Noguchi and Kohei Uosaki*

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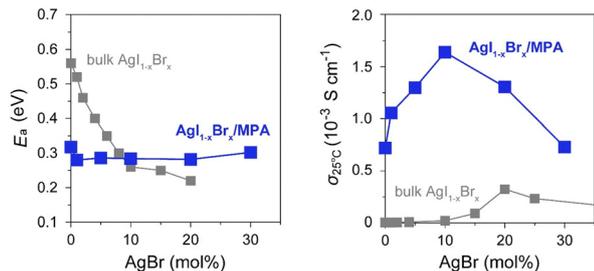


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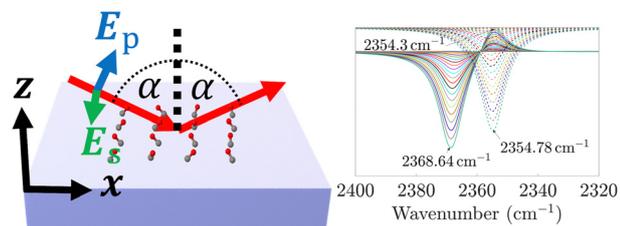
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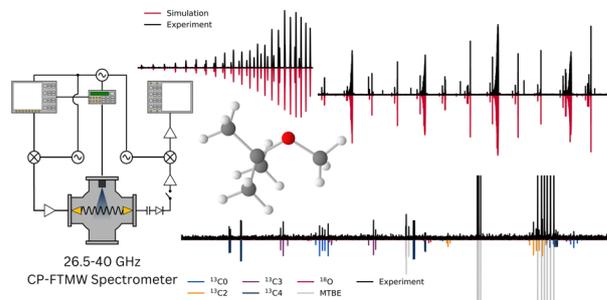


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Rotational spectroscopy of methyl *tert*-butyl ether with a new K_a band chirped-pulse Fourier transform microwave spectrometer

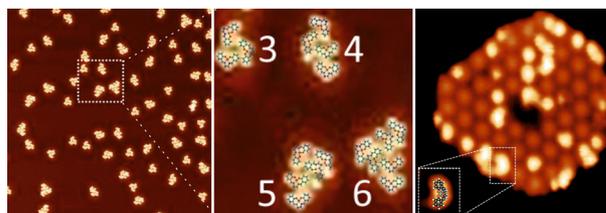
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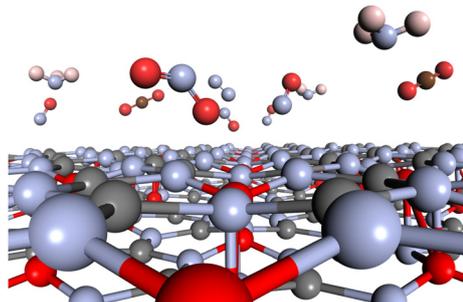
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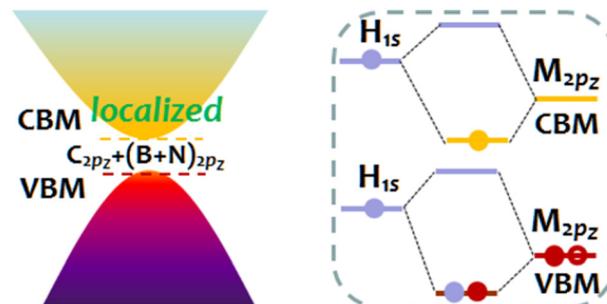
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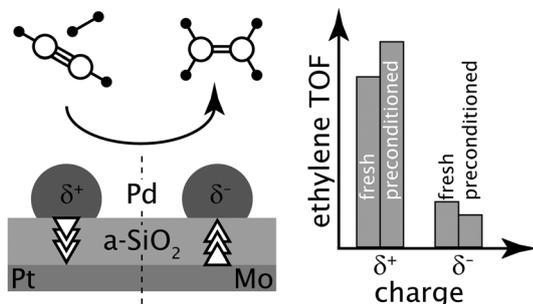
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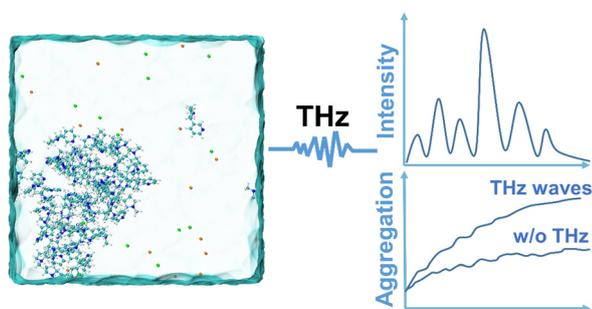
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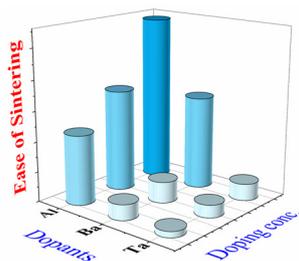
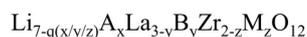
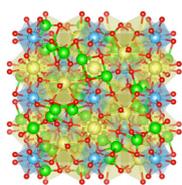
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Effect of terahertz waves on the aggregation behavior of neurotransmitters

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

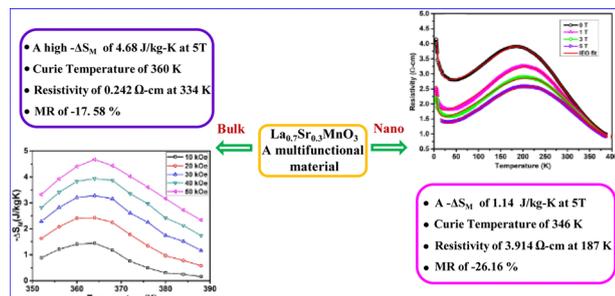
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First-principles evaluation of dopant impact on structural deformability and processability of $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$

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

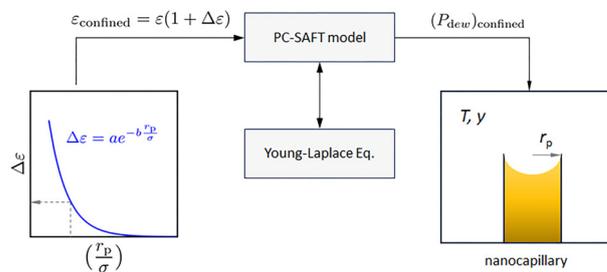


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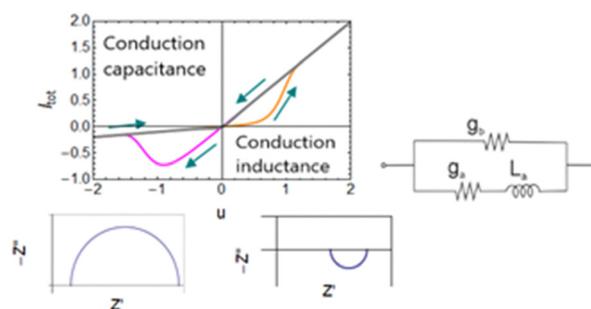
Aliakbar Roosta, Sohrab Zendehboudi and Nima Rezaei*



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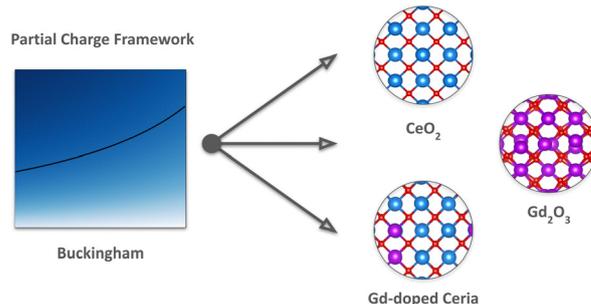
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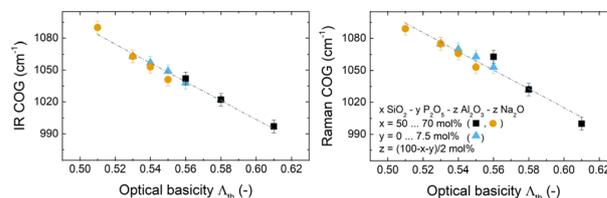
Josef M. Gallmetzer, Jakob Gamper, Felix R. S. Purtscher and Thomas S. Hofer*



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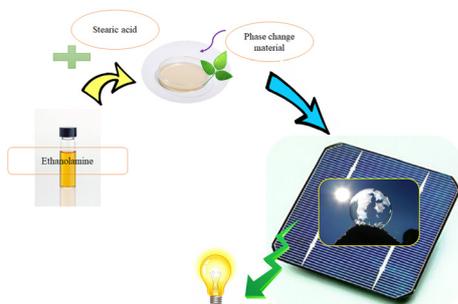
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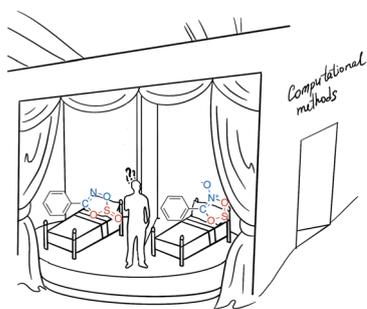
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Thermal properties of novel phase change materials based on protic ionic liquids containing ethanolamines and stearic acid for efficient thermal energy storage

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

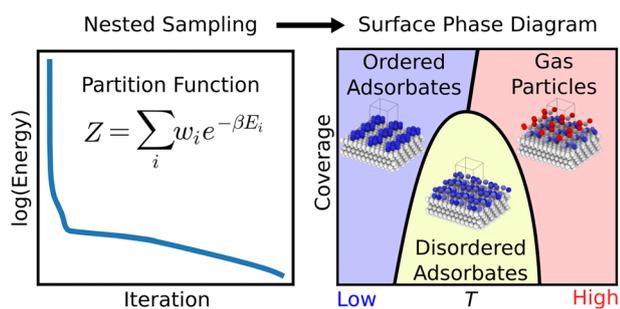
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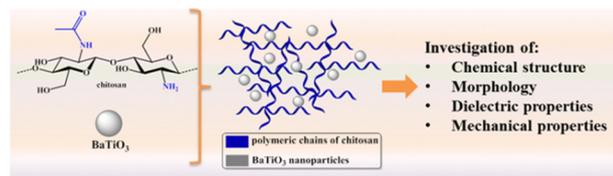
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Surface phase diagrams from nested sampling

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

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Biophysical stimulation for bone regeneration using a chitosan/barium titanate ferroelectric composite

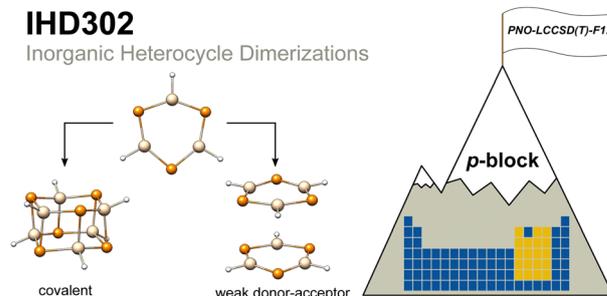
Razvan Rotaru, Violeta Melinte and Ioana-Sabina Trifan*



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The p-block challenge: assessing quantum chemistry methods for inorganic heterocycle dimerizations

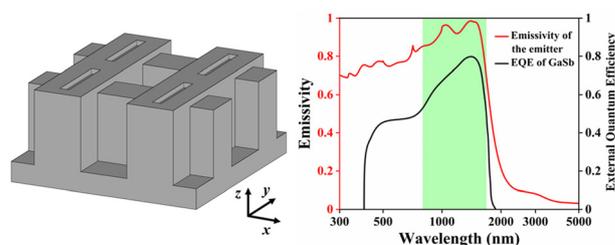
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A tungsten-based metamaterial emitter for solar thermophotovoltaic systems

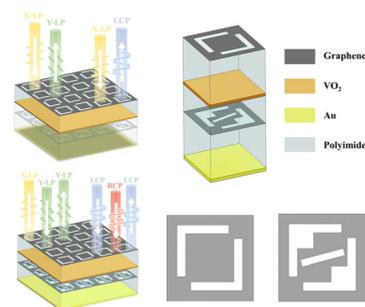
Yuchun Cao,* Heng Zhang, Ning Chen, Haotuo Liu, Yongtao Feng and Xiaohu Wu*



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Tunable and switchable multifunctional terahertz meta-mirror based on graphene and vanadium dioxide

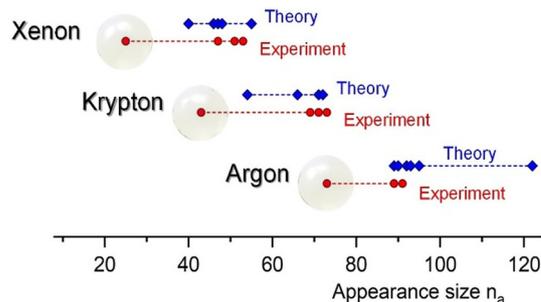
Xinzhi Zhang, Aihui Sun, Zhilong Jiang, Cheng Liu, Shouyu Wang and Yan Kong*



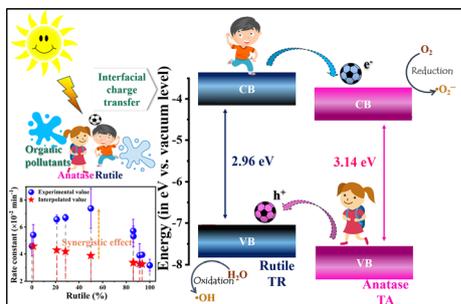
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Size limits and fission channels of doubly charged noble gas clusters

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



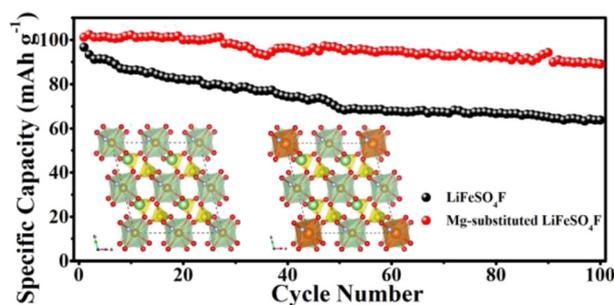
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Band alignment and interfacial charge transfer in sol-gel derived anatase/rutile heterophase TiO₂: explaining the synergistic photocatalytic activity

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

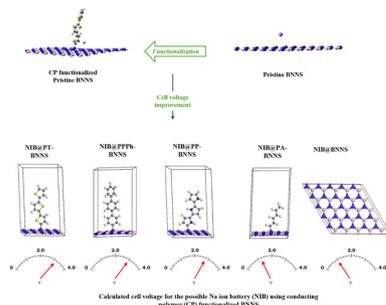
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Improved structure stability and performance of a LiFeSO₄F cathode material for lithium-ion batteries by magnesium substitution

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

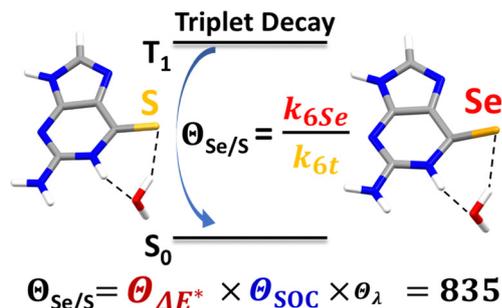
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Anodic voltage performance of conducting polymer-functionalized boron nitride nanosheets: a DFT assessment

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

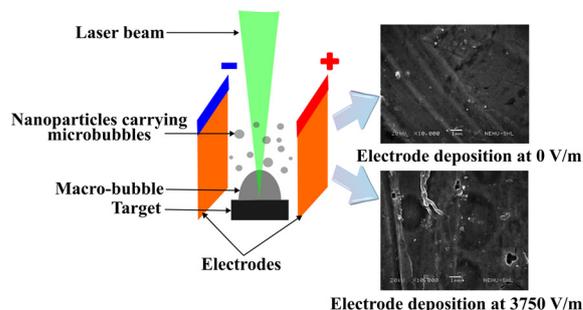
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Bubble-assisted microstreaming during electrode deposition of Mn_2O_3 energy harvesters

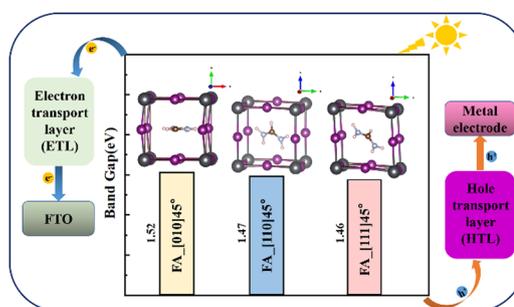
Sanchia Mae Kharphanbuh, Prahlad K. Baruah, Alika Khare and Arpita Nath*



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

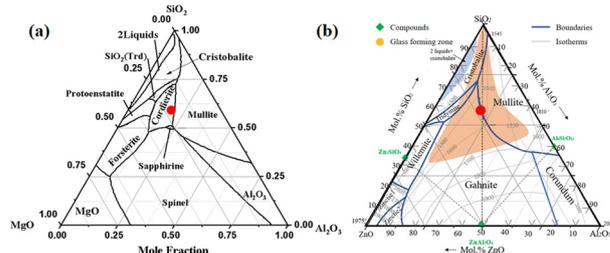
Shuning Wang, Qi Yang, Xiuchen Han, Dongmeng Chen, Bing Liu and Wenjing Fang*



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

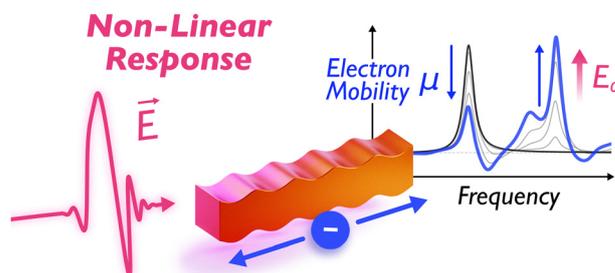
Biwei Huang, Qingshuang Zheng, Muzhi Cai, Ang Qiao and Haizheng Tao*



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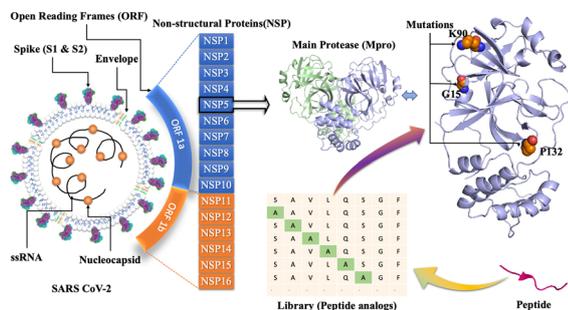
Field-dependent THz transport nonlinearities in semiconductor nano structures

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



RESEARCH PAPERS

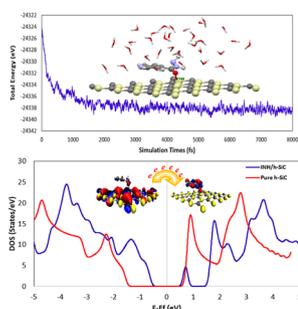
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De novo design of potential peptide analogs against the main protease of Omicron variant using *in silico* studies

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

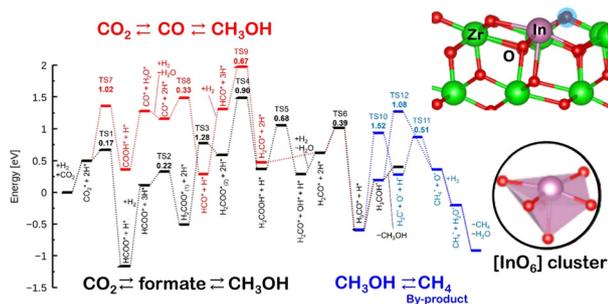
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Unravelling performance of honeycomb structures as drug delivery systems for the izoniazid drug using DFT-D3 correction dispersion and molecular dynamic simulations

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

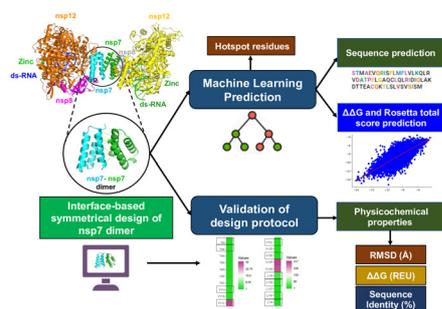
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Difference in reaction mechanism between ZnZrO_x and InZrO_x for CO₂ hydrogenation

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

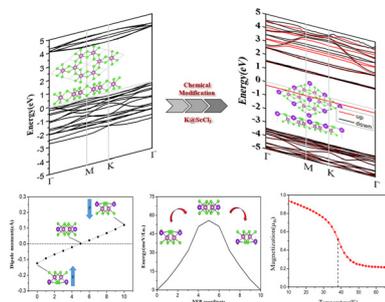
Amar Jeet Yadav, Shivank Kumar, Shweeta Maurya, Khushboo Bhagat and Aditya K. Padhi*



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

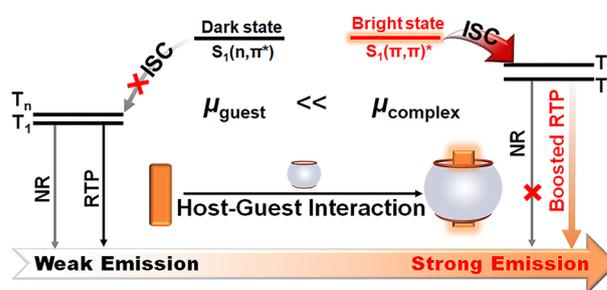
Yu Liang, Huasheng Sun, Xiang Li, Leichuang Zhu, Menghao Bi, Zhengxiao Du, Chengxi Huang* and Fang Wu*



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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*

