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IN THIS ISSUE

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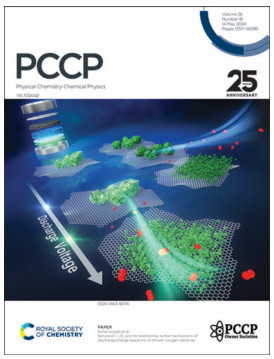

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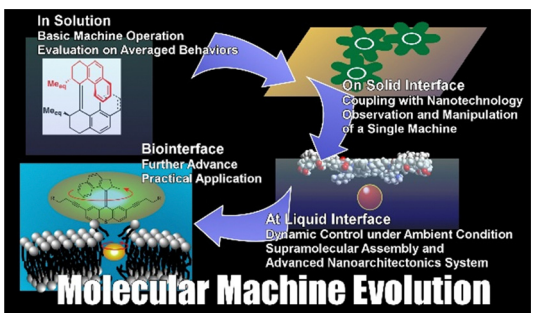

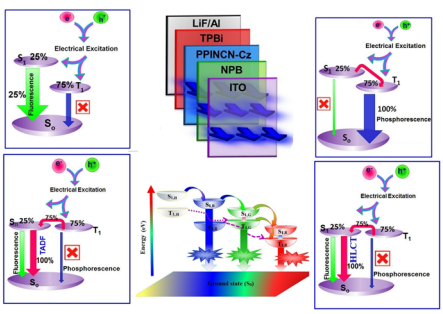

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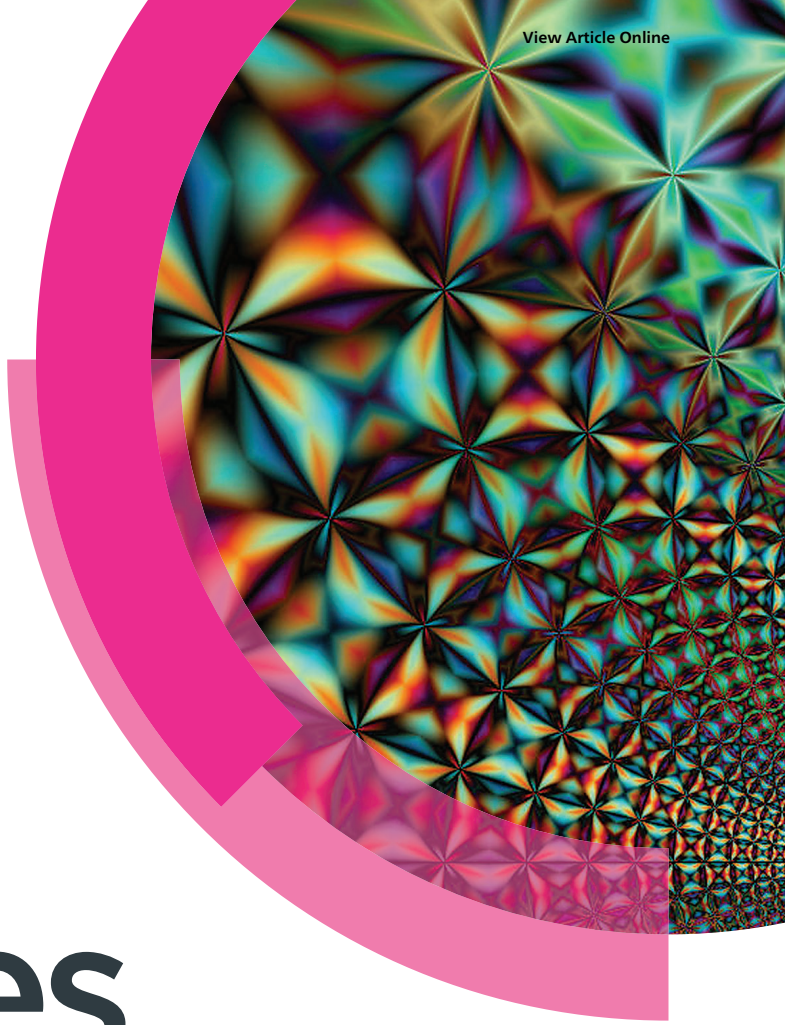

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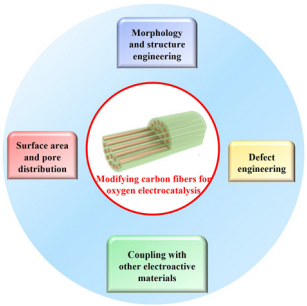

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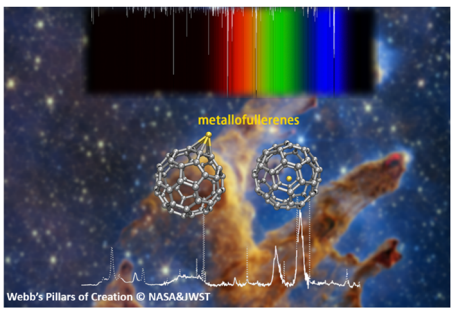

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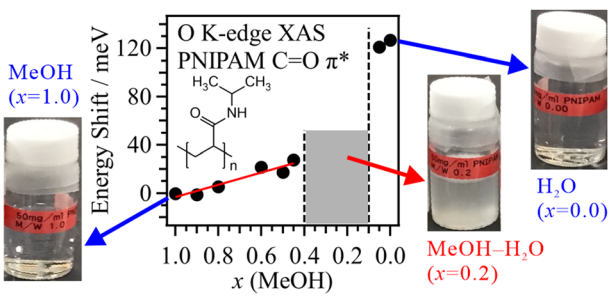

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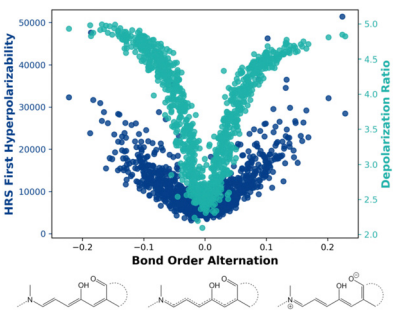

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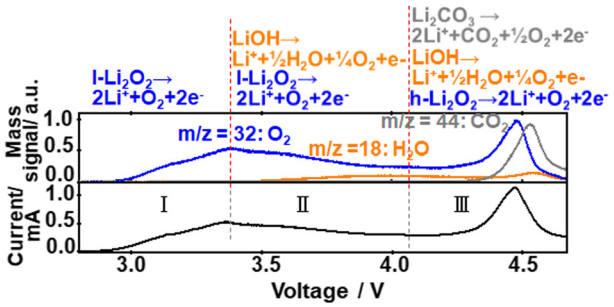
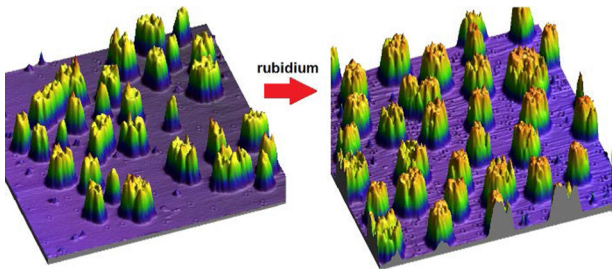


Nature of Li_2O_2 and its relationship to the mechanisms of discharge/charge reactions of lithium–oxygen batteries

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

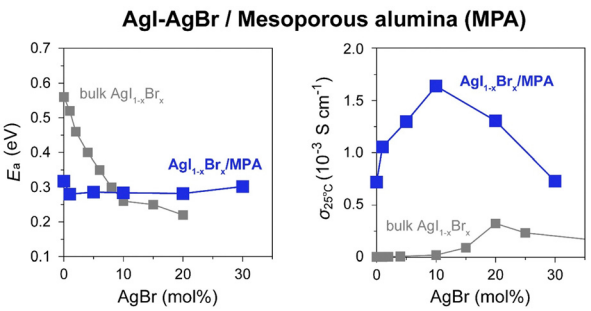
13667



The structure-giving role of Rb^+ ions for water–ice nanoislands supported on Cu(111)

Javier A. Martínez,* Inga C. Langguth, David Olivenza-León and Karina Morgenstern

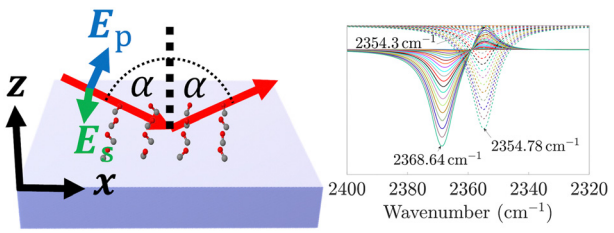
13675



Systematic study of ionic conduction in silver iodide/mesoporous alumina composites 2: effects of silver bromide doping

Yoko Fukui,* Yukihiro Yoshida,* Hiroshi Kitagawa and Yohei Jikihara

13683



Polarization-dependent effects in vibrational absorption spectra of 2D finite-size adsorbate islands on dielectric substrates

Benedikt Zerulla,* Marjan Krstić, Shuang Chen, Zairan Yu, Dominik Beutel, Christof Holzer, Markus Nyman, Alexei Nefedov, Yuemin Wang, Thomas G. Mayerhöfer, Christof Wöll* and Carsten Rockstuhl*

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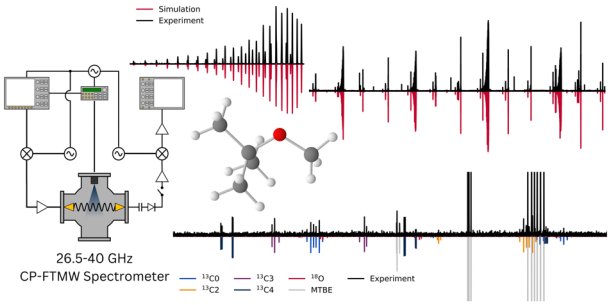

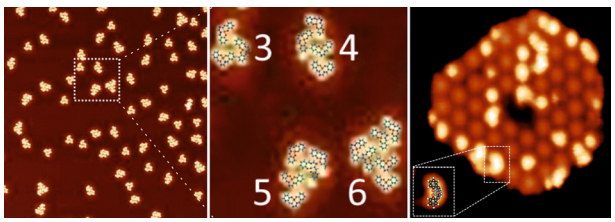

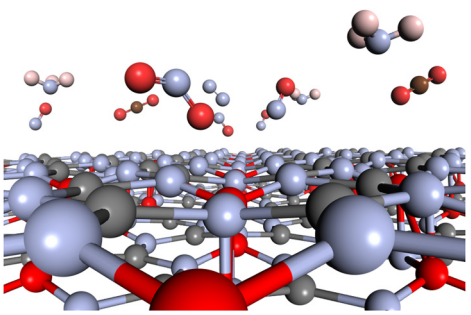

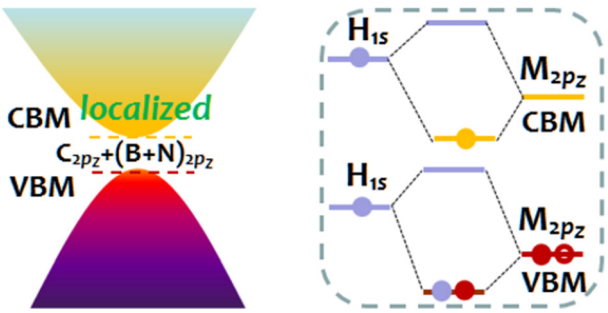

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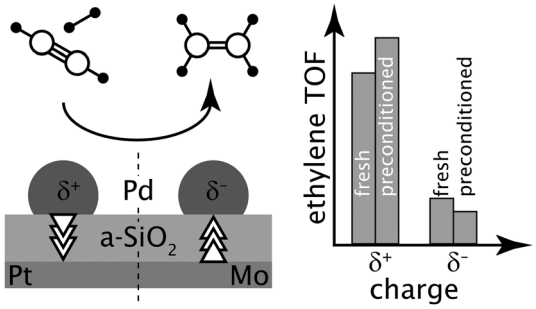
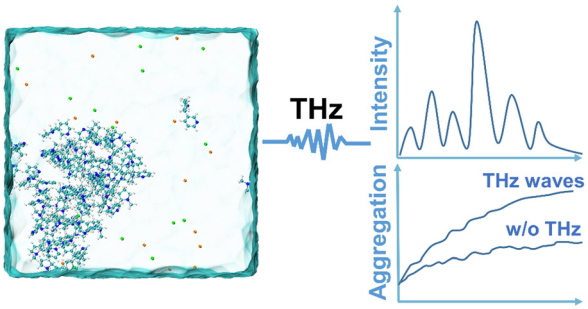


Same size, same support, same spectator? Selective acetylene hydrogenation on supported Pd nanoparticles

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

13751



Effect of terahertz waves on the aggregation behavior of neurotransmitters

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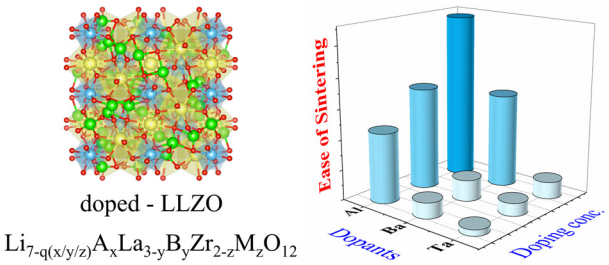
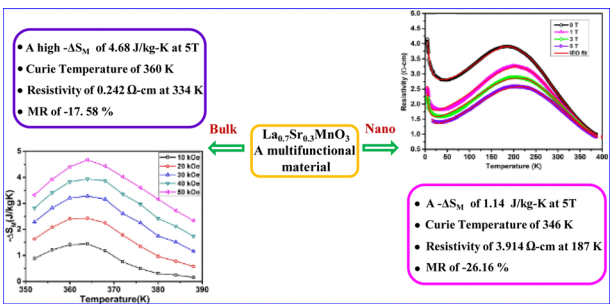
13762



First-principles evaluation of dopant impact on structural deformability and processability of $Li_7La_3Zr_2O_{12}$

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

13773



Investigation on the structural, magnetic, magnetocaloric and magnetotransport behaviour of $La_{0.7}Sr_{0.3}MnO_3$ manganites synthesised by different routes

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

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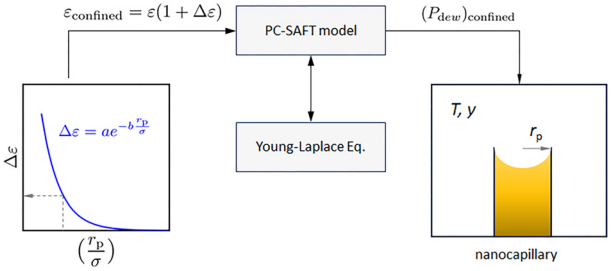

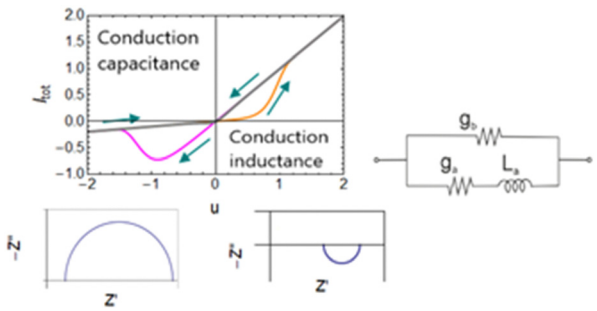

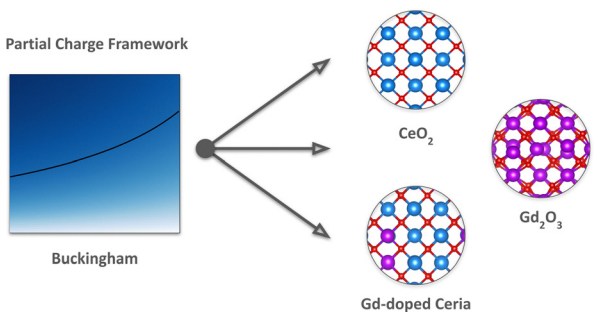

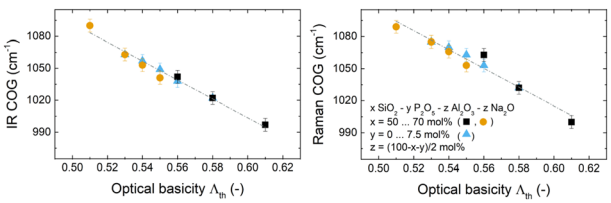

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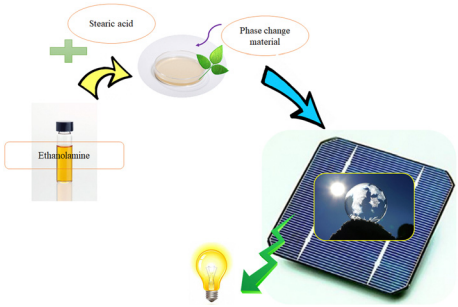
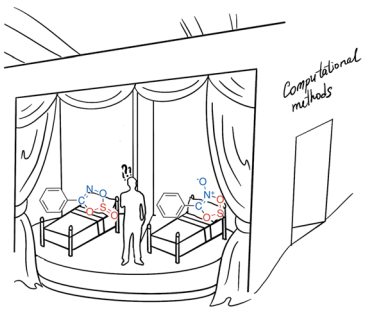


Thermal properties of novel phase change materials based on protic ionic liquids containing ethanolamines and stearic acid for efficient thermal energy storage

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

13850



From a humorous post to a detailed quantum-chemical study: isocyanate synthesis revisited

Oleg B. Beletsan, Igor Gordiy, Sergey S. Lunkov, Mikhail A. Kalinin, Larisa E. Alkhimova, Egor A. Nosach, Egor A. Ilin, Alexandr V. Bespalov, Olgert L. Dallakyan, Aleksandr A. Chamkin, Ilya V. Prolomov, Radion A. Zaripov, Andrey A. Pershin, Bogdan O. Protsenko, Yury V. Rusalev, Ruslan A. Oganov, Diana K. Kovaleva, Vladimir A. Mironov, Victor V. Dotsenko, Alexandr M. Genaev,* Dmitry I. Sharapa* and Denis S. Tikhonov*

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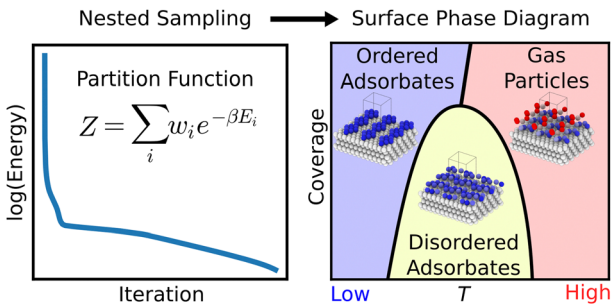
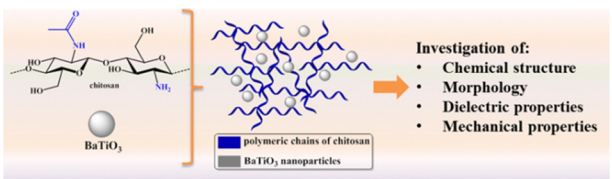


Surface phase diagrams from nested sampling

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

13875



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

Razvan Rotaru, Violeta Melinte and Ioana-Sabina Trifan*

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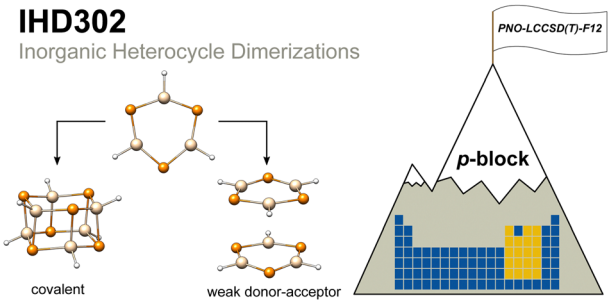

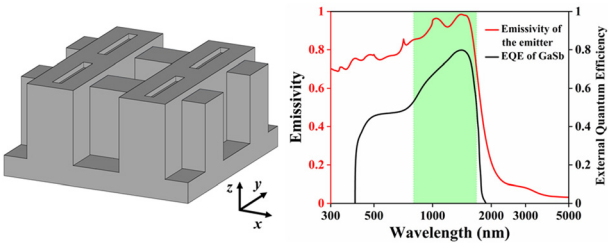

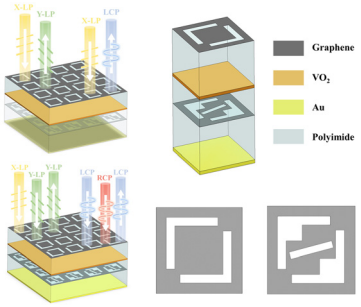

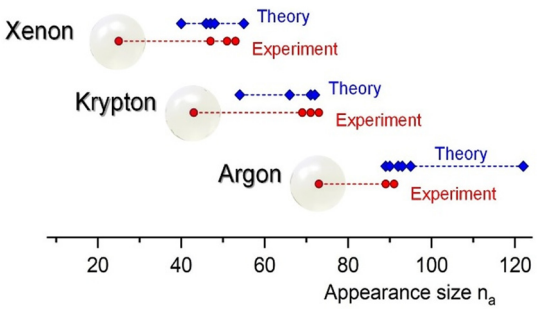

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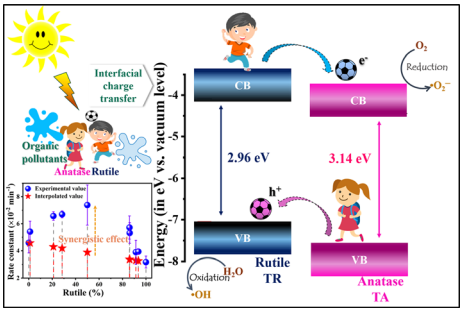
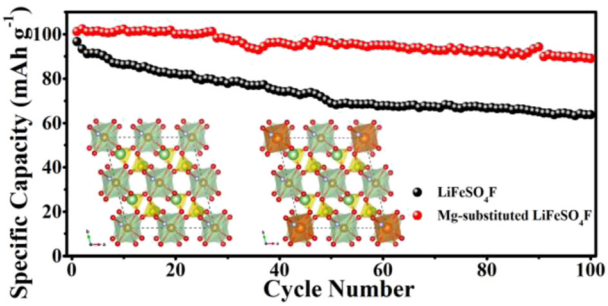


Band alignment and interfacial charge transfer in sol–gel derived anatase/rutile heterophase TiO_2: explaining the synergistic photocatalytic activity

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

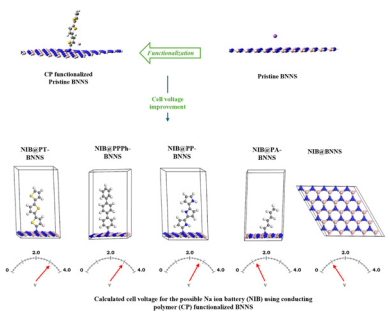
13949



Improved structure stability and performance of a $LiFeSO_4F$ cathode material for lithium-ion batteries by magnesium substitution

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

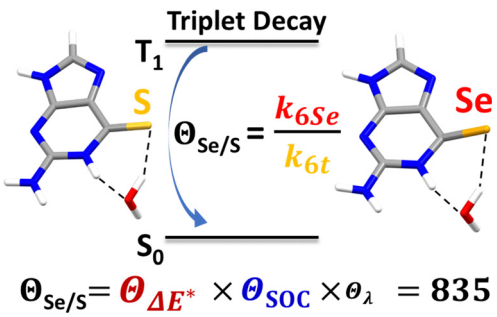
13955



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

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

13965



Unexpected longer T_1 lifetime of 6-sulfur guanine than 6-selenium guanine: the solvent effect of hydrogen bonds to brake the triplet decay

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

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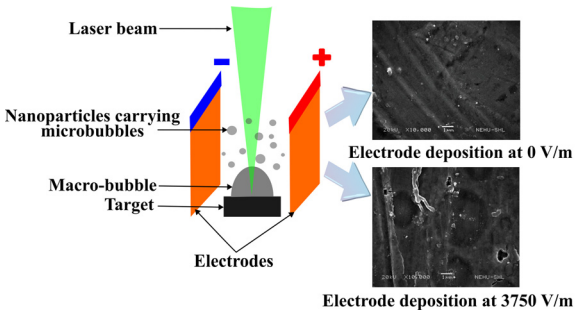

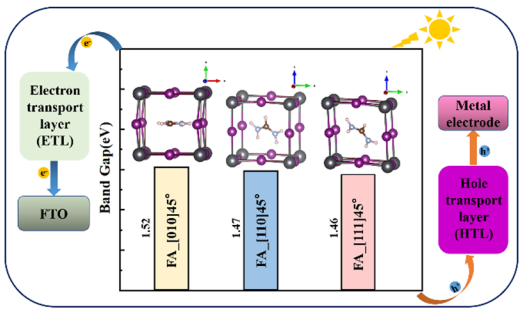

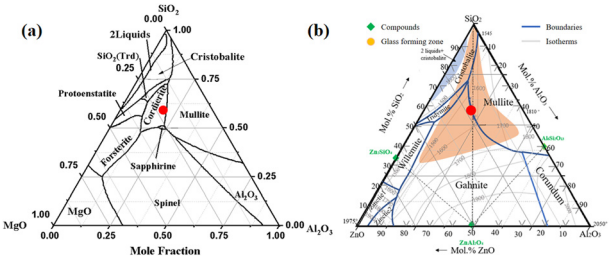

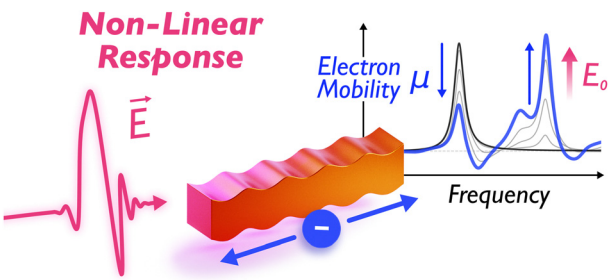

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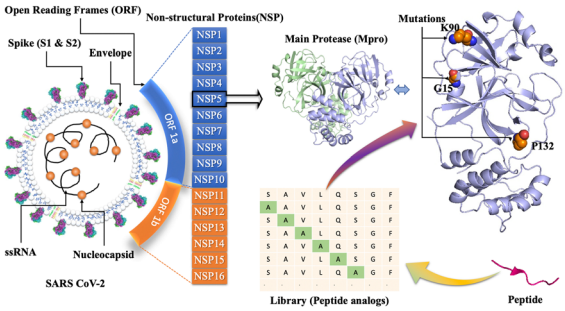
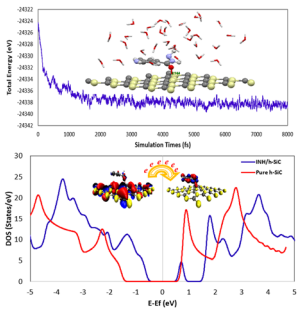


De novo design of potential peptide analogs against the main protease of Omicron variant using *in silico* studies

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

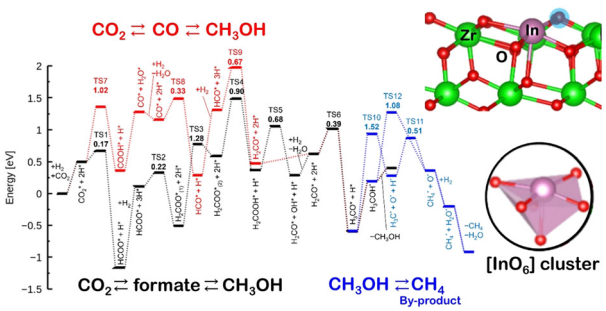
14018



Unravelling performance of honeycomb structures as drug delivery systems for the isoniazid 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*

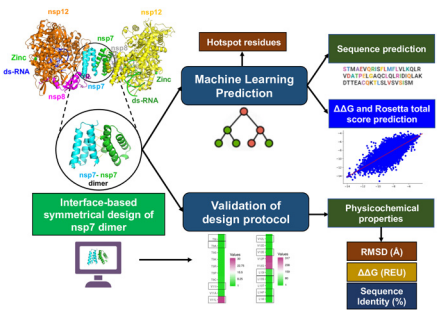
14037



Difference in reaction mechanism between $ZnZrO_x$ and $InZrO_x$ for CO_2 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, Shweata Maurya, Khushboo Bhagat and Aditya K. Padhi*

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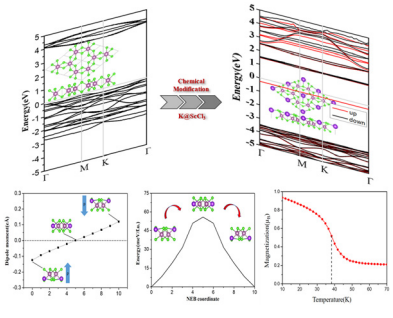

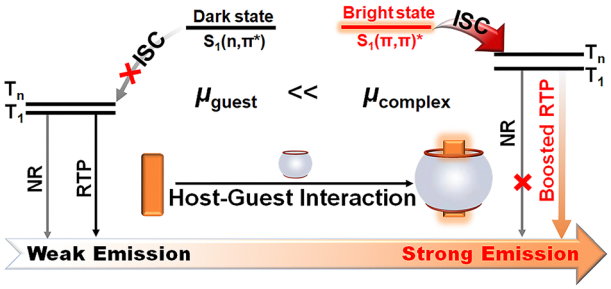

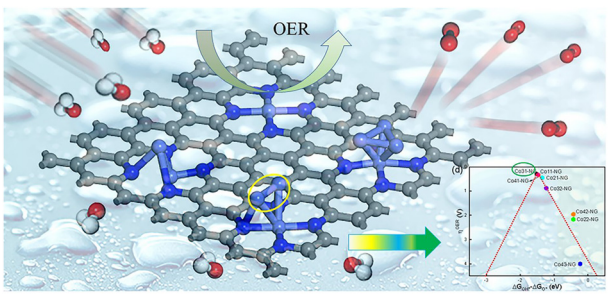

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