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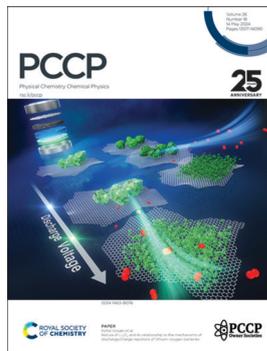
IN THIS ISSUE

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Cover

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Inside cover

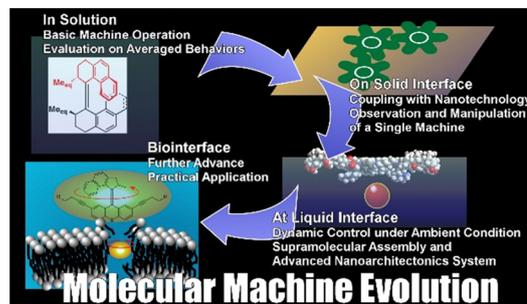
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REVIEWS

13532

Molecular machines working at interfaces: physics, chemistry, evolution and nanoarchitectonics

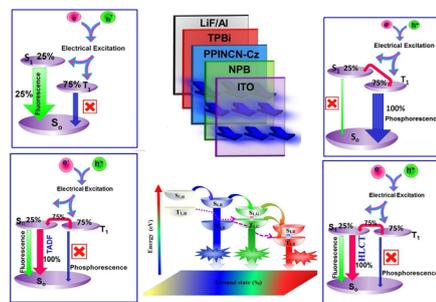
Katsuhiko Ariga,* Jingwen Song and Kohsaku Kawakami



13561

Robust luminogens as cutting-edge tools for efficient light emission in recent decades

Jayaraman Jayabharathi* and Venugopal Thanikachalam



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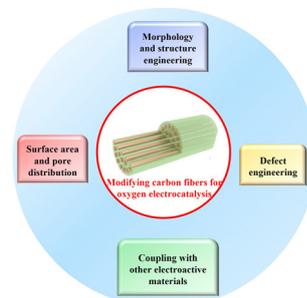


REVIEWS

13606

Modification of carbon nanofibers for boosting oxygen electrocatalysis

Changming Ding, Yitao Zhao* and Zhiyong Qiao*

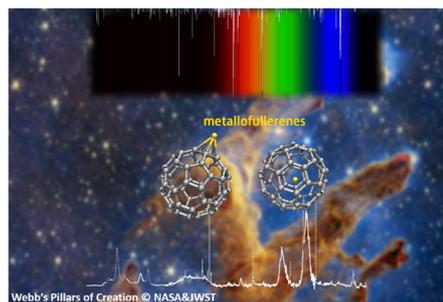


PERSPECTIVE

13622

Metallofullerenes as potential candidates for the explanation of astrophysical phenomena

Ransel Barzaga* and Gao-Lei Hou*

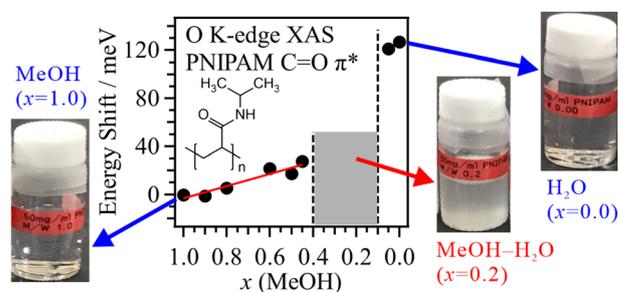


COMMUNICATION

13634

Mechanism of poly(*N*-isopropylacrylamide) cononsolvency in aqueous methanol solutions explored *via* oxygen K-edge X-ray absorption spectroscopy

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

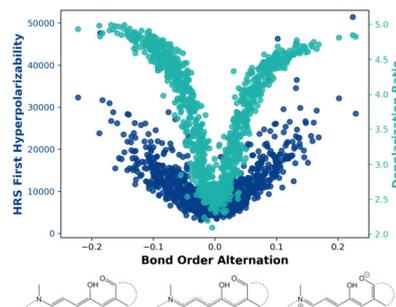


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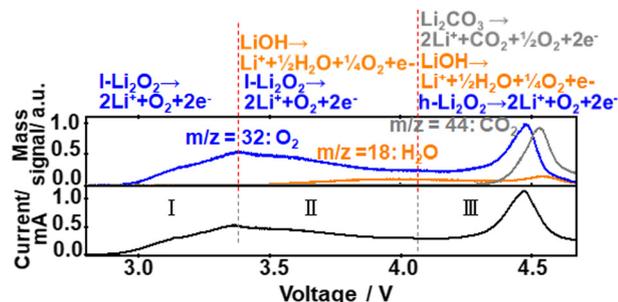
13639

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*



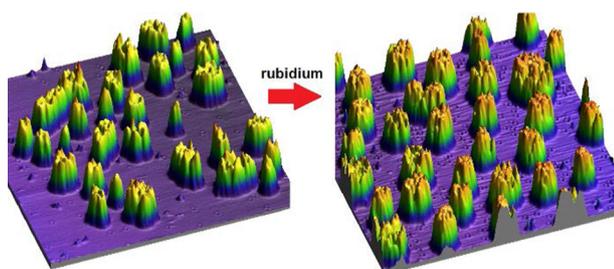
13655



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

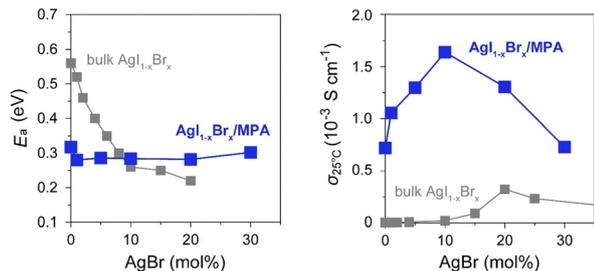


The structure-giving role of Rb^+ ions for water–ice nanoislands supported on Cu(111)

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

13675

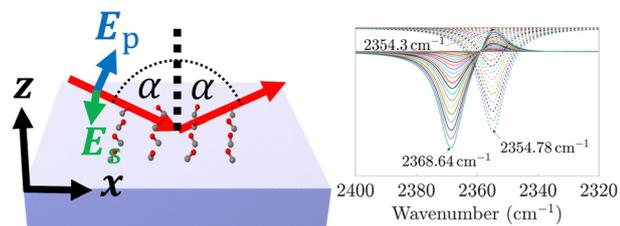
AgI–AgBr / Mesoporous alumina (MPA)



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*

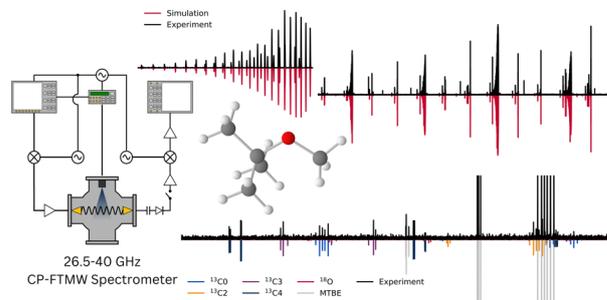


RESEARCH PAPERS

13694

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

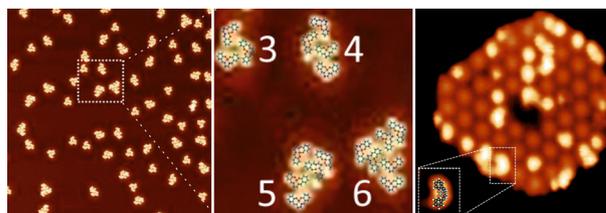
Kyle N. Crabtree,* J. H. Westerfield, Chisom A. Dim, Kelly S. Meyer, Sommer L. Johansen, Zachary S. Buchanan and Paul A. Stucky



13710

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

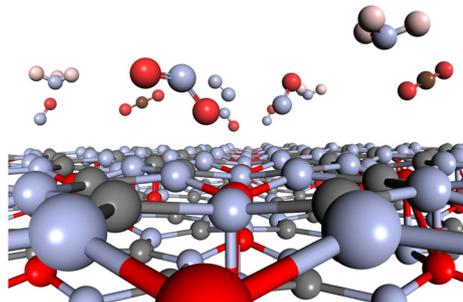
Sigmund Jensen, Isaac Appelquist Løge, Jesper Bendix and Lars Diekhöner*



13719

Atomic insights into the interaction of N_2 , CO_2 , NH_3 , NO , and NO_2 gas molecules with $\text{Zn}_2(\text{V}, \text{Nb}, \text{Ta})\text{N}_3$ ternary nitride monolayers

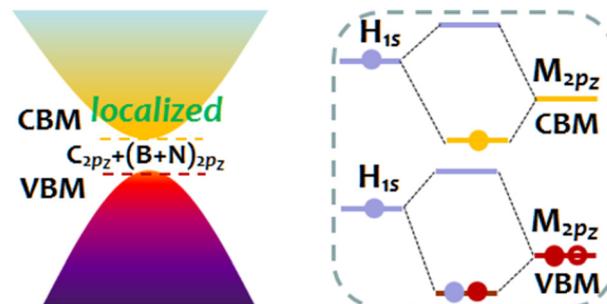
Andrey A. Kistanov



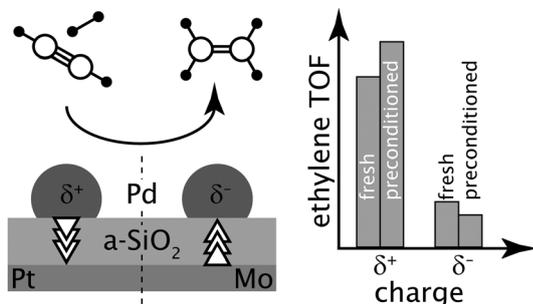
13731

Enhancing the energetic and magnetic stability of atomic hydrogen chemisorbed on graphene using (non)compensated B–N pairs

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



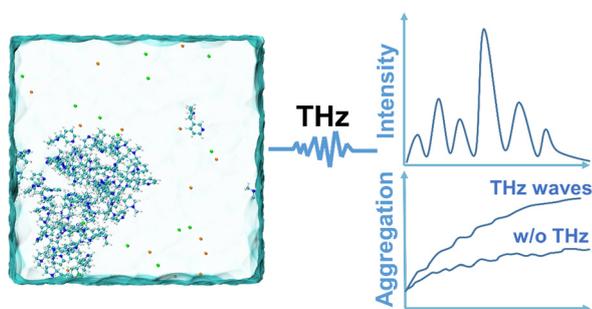
13740



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*

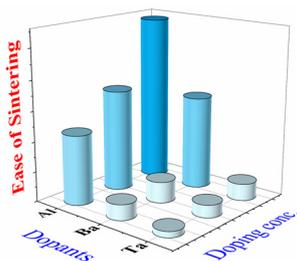
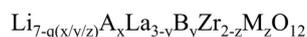
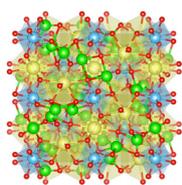
13751



Effect of terahertz waves on the aggregation behavior of neurotransmitters

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

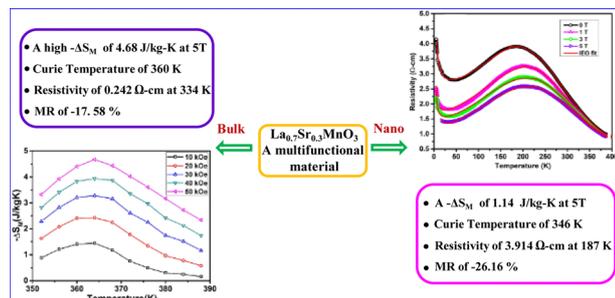
13762



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*

13773



Investigation on the structural, magnetic, magnetocaloric and magnetotransport behaviour of $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ manganites synthesised by different routes

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

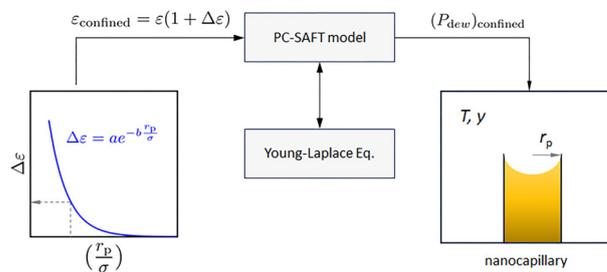


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13790

Improving the estimation accuracy of confined vapor–liquid equilibria by fine-tuning the pure component parameter in the PC-SAFT equation of state

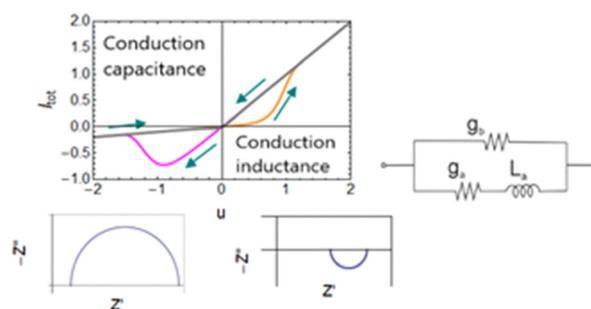
Aliakbar Roosta, Sohrab Zendeboudi and Nima Rezaei*



13804

Hysteresis in memristors produces conduction inductance and conduction capacitance effects

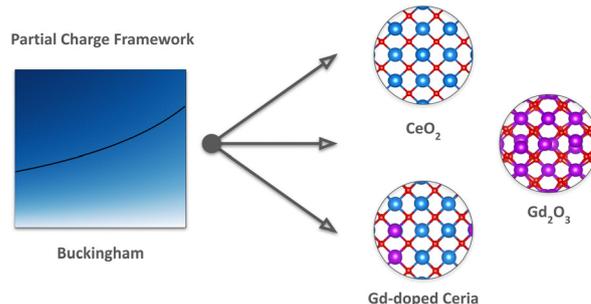
Juan Bisquert,* Juan B. Roldán and Enrique Miranda



13814

Modelling bulk and surface characteristics of cubic CeO_2 , Gd_2O_3 , and gadolinium-doped ceria using a partial charge framework

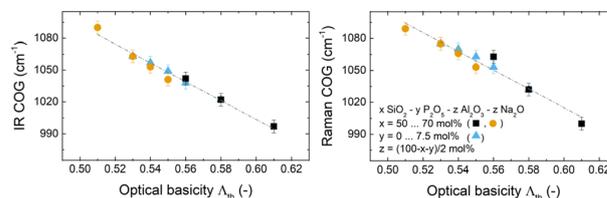
Josef M. Gallmetzer, Jakob Gamper, Felix R. S. Purtscher and Thomas S. Hofer*



13826

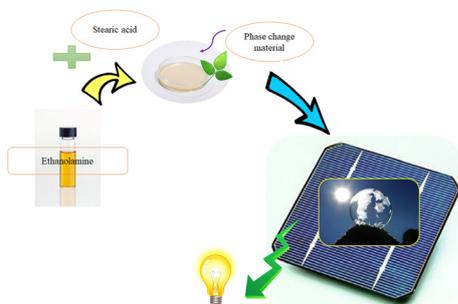
Dispersion, ionic bonding and vibrational shifts in phospho-aluminosilicate glasses

Thilo Grammes, Dominique de Ligny, Dintu Mathew, Kristin Griebenow, Franziska Scheffler, Florian Lindner, Claudia Aichele, Jan Dellith, Leo van Wüllen, Efstratios I. Kamitsos* and Delia S. Brauer*



RESEARCH PAPERS

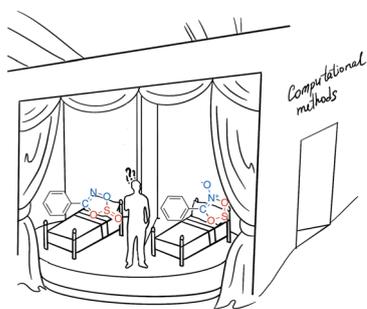
13839



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

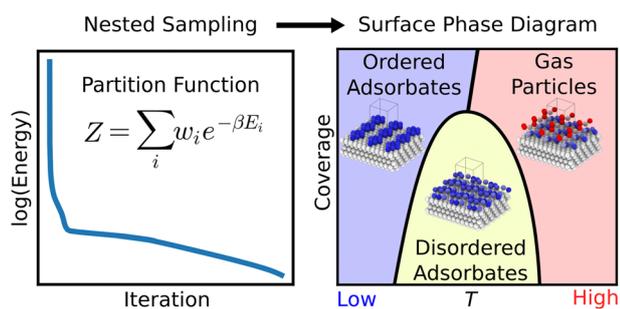
13850



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

Oleg B. Beletskiy, 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*

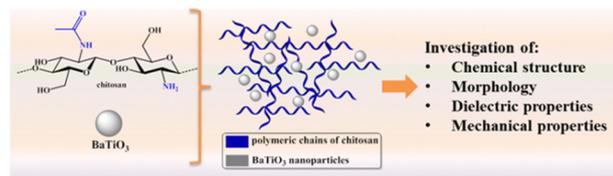
13862



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

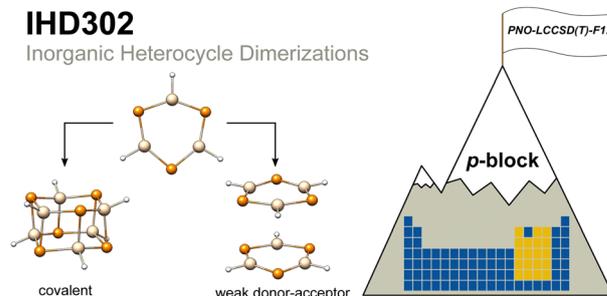
Razvan Rotaru, Violeta Melinte and Ioana-Sabina Trifan*



13884

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

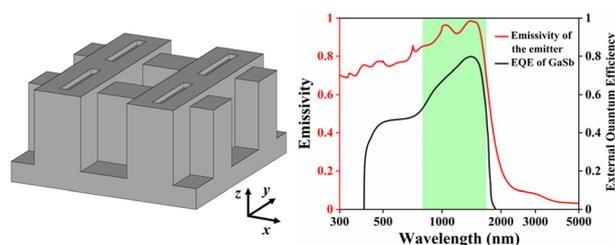
Thomas Gasevic, Markus Bursch,* Qianli Ma, Stefan Grimme, Hans-Joachim Werner* and Andreas Hansen*



13909

A tungsten-based metamaterial emitter for solar thermophotovoltaic systems

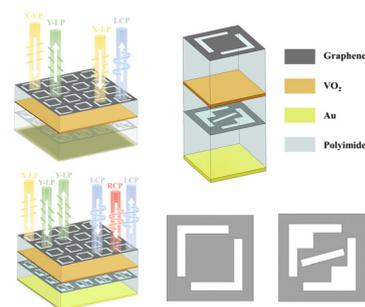
Yuchun Cao,* Heng Zhang, Ning Chen, Haotuo Liu, Yongtao Feng and Xiaohu Wu*



13915

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

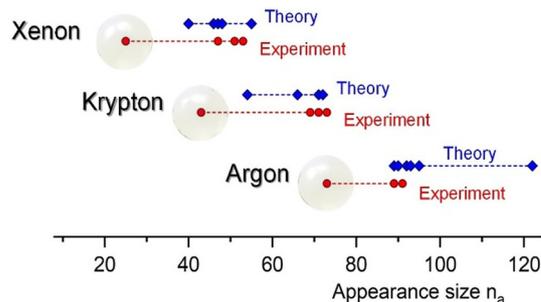
Xinzhi Zhang, Aihui Sun, Zhilong Jiang, Cheng Liu, Shouyu Wang and Yan Kong*



13923

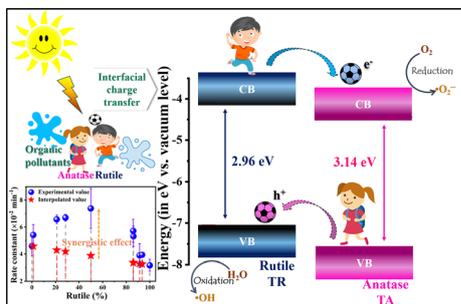
Size limits and fission channels of doubly charged noble gas clusters

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



RESEARCH PAPERS

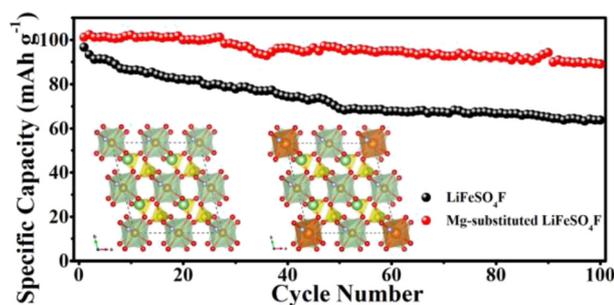
13937



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.*

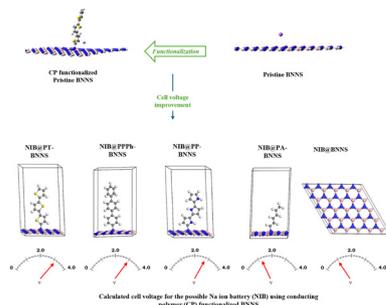
13949



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*

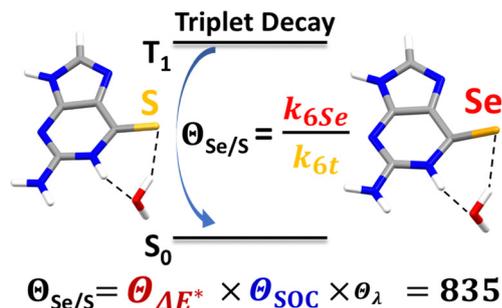
13955



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*

13965



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

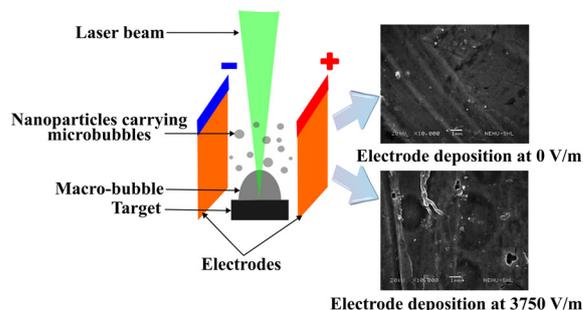
Shaoting Liu, Yuhuan Lee, Lingfang Chen, Jingheng Deng, Tongmei Ma,* Mario Barbatti* and Shuming Bai*



13973

Bubble-assisted microstreaming during electrode deposition of Mn_2O_3 energy harvesters

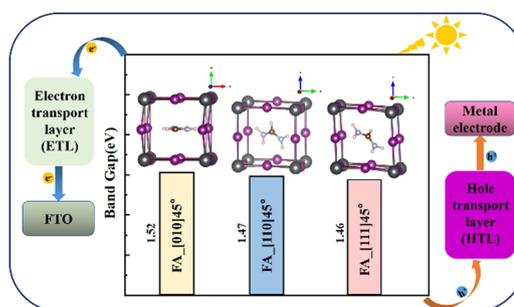
Sanchia Mae Kharphanbuh, Prahlad K. Baruah, Alika Khare and Arpita Nath*



13979

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

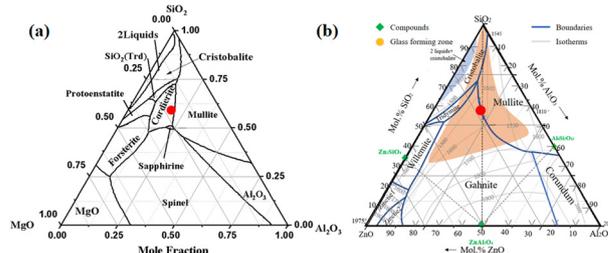
Shuning Wang, Qi Yang, Xiuchen Han, Dongmeng Chen, Bing Liu and Wenjing Fang*



13987

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

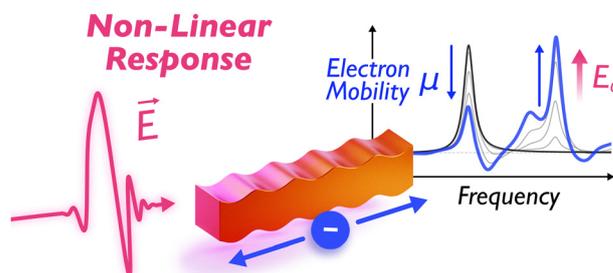
Biwei Huang, Qingshuang Zheng, Muzhi Cai, Ang Qiao and Haizheng Tao*



13995

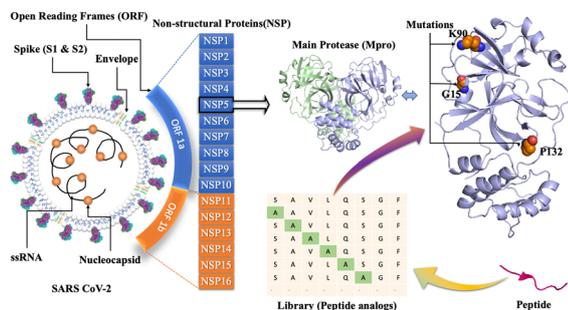
Field-dependent THz transport nonlinearities in semiconductor nano structures

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



RESEARCH PAPERS

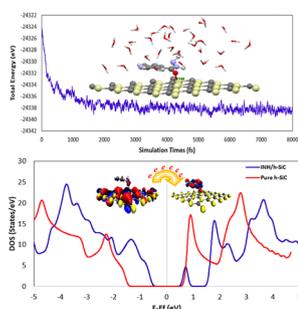
14006



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.*

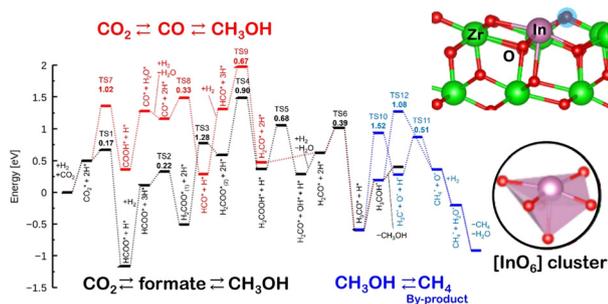
14018



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

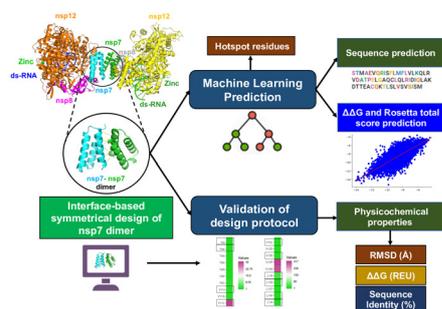
14037



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*

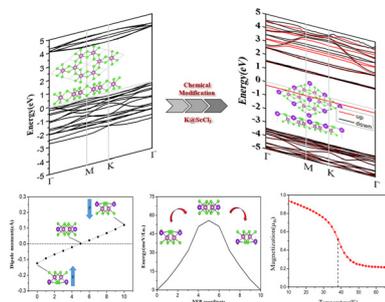


RESEARCH PAPERS

14062

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

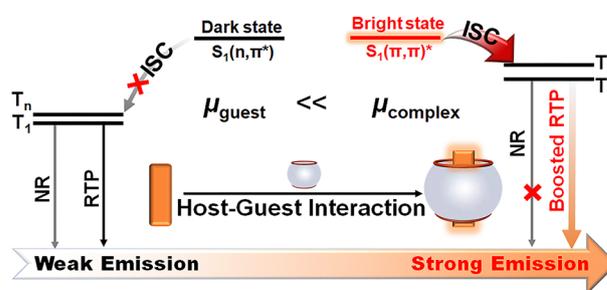
Yu Liang, Huasheng Sun, Xiang Li, Leichuang Zhu, Menghao Bi, Zhengxiao Du, Chengxi Huang* and Fang Wu*



14071

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

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



14079

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*

