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Cover

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EDITORIAL

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Size effects in chemistry & physics of atomic & molecular clusters, nanoparticles & nanostructures

André Fielicke, Sandra M. Lang and Thorsten M. Bernhardt

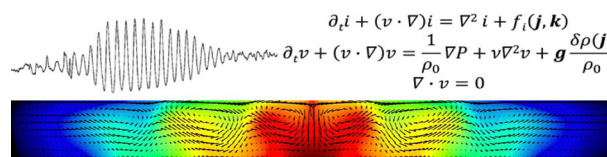


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Transport-driven chemical oscillations: a review

M. A. Budroni* and F. Rossi



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PERSPECTIVE

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Breaking the Brownian barrier: models and manifestations of molecular diffusion in complex fluids

Harish Srinivasan,* Veerendra K. Sharma* and Subhankur Mitra

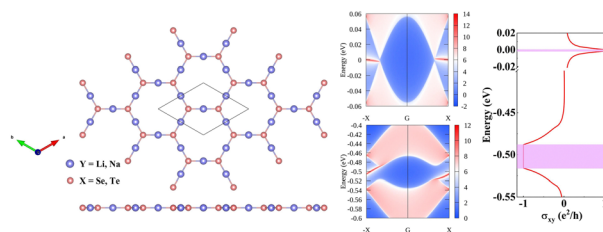


COMMUNICATION

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The quantum anomalous Hall effect and strong robustness in two-dimensional p-state Dirac half-metals Y_3X_2 ($Y = \text{Li, Na}$; $X = \text{Se, Te}$)

Ao Du, Yanghao Tang, Long Kuang, Shi Qiu, Ting Yang, Jinming Cai* and Cuixia Yan*

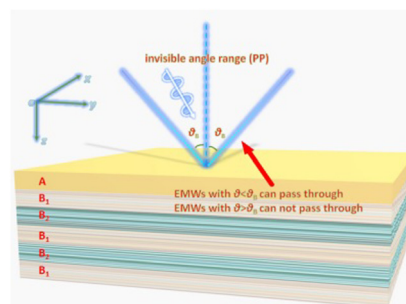


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A layered metastructure for privacy protection based on the Brewster angle

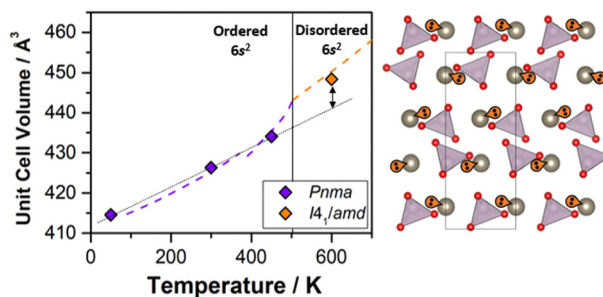
Hao-Ran Xu, Bao-Fei Wan and Hai-Feng Zhang*



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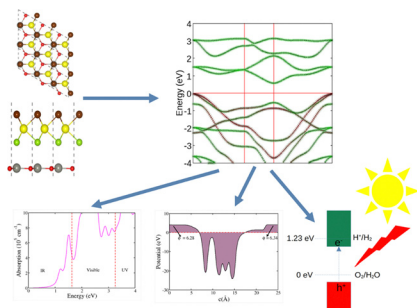
Toxic, radioactive, and disordered: a total scattering study of TlTcO_4

Bryce G. Mullens, Frederick P. Marlton,* Matilde Saura-Múzquiz, Michelle Everett, Cheng Li, Alicia M. Manjon-Sanz, Matthew G. Tucker, Frederic Poineau, James Louis-Jean, Supratik Mukherjee, Subrata Mondal, Ganapathy Vaitheeswaran* and Brendan J. Kennedy



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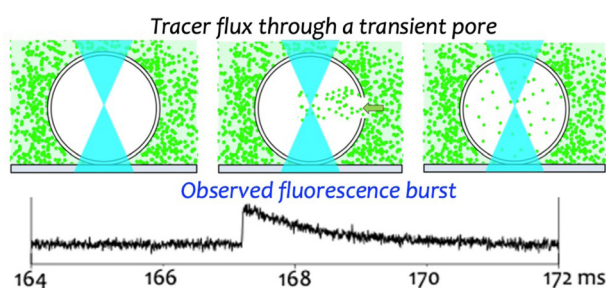
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First principles study of photocatalytic activity in ZnO-Janus van der Waals heterostructures

Tahir Wahab,* Antonio Cammarata* and Tomas Polcar

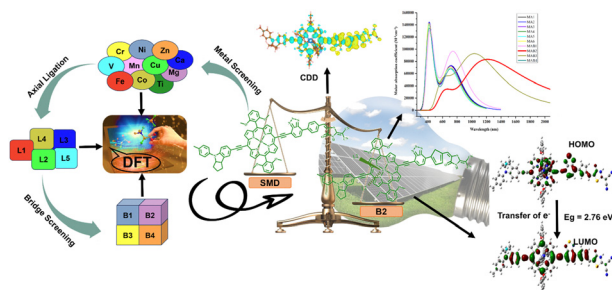
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Nanoscope spontaneous poration as a precursor to protein-based transport in early protocells

Tai-You Chu, Chia-Hsuan Lee, Minh Thuy Vo and Ian Liao*

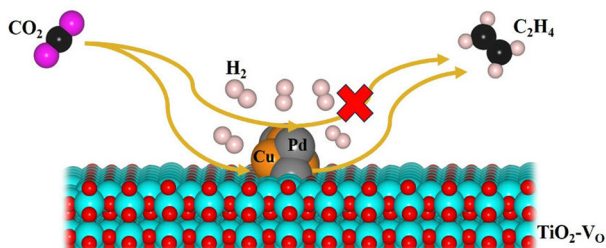
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Engineering highly efficient porphyrin sensitizers through metal, ligand and bridge modification: a DFT study

Hemjot Kaur and Neetu Goel*

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Effects of surface oxygen vacancy on CO₂ adsorption and its activation towards C₂H₄ using metal (Cu, Pd, CuPd) cluster-loaded TiO₂ catalysts: a first principles study

Sajjad Hussain, Lina Zhang, Zhengzheng Xie,* Jianjun Yang and Qiuye Li*

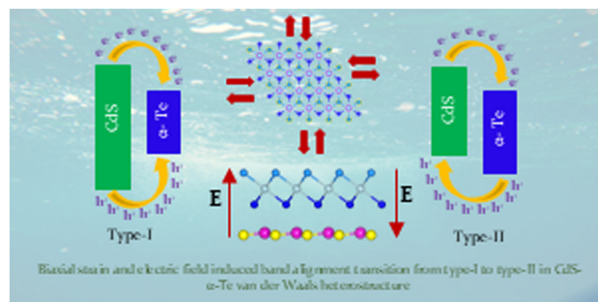


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Band alignment in CdS- α -Te van der Waals heterostructures for photocatalytic applications: influence of biaxial strain and electric field

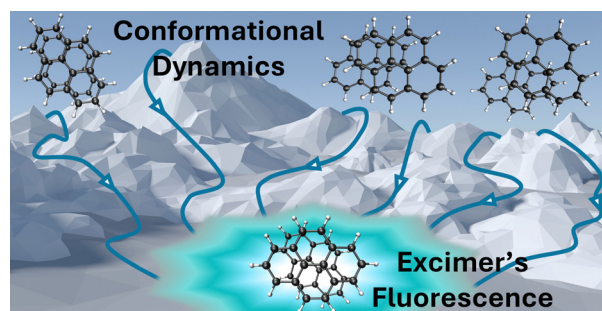
G. Tejaswini, Anjana E. Sudheer, M. Vallinayagam, M. Posselt, M. Zschornak, S. Maniprakash and D. Murali*



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Conformational dynamics of the pyrene excimer

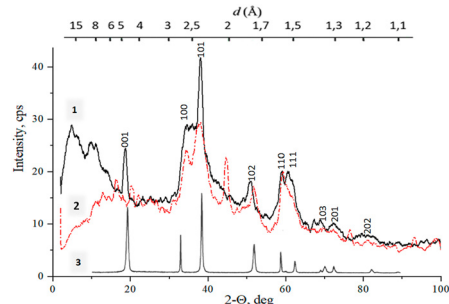
Giovanni Parolin, Bidhan Chandra Garain, Saikat Mukherjee, Giovanni Granucci, Stefano Corni and Mario Barbatti*



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Investigation of oxidation–reduction processes of nickel hydroxide precipitation and their carbothermal reduction

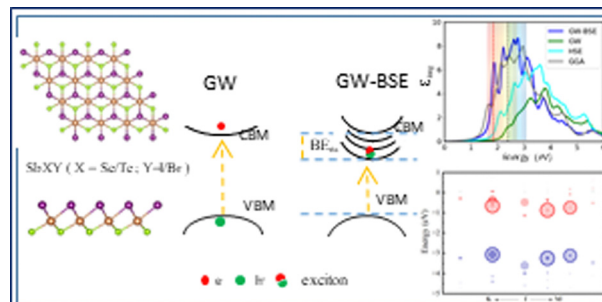
Viktoriia Bohatyrenko, Dmytro Kamenskyh, Maarif Jafarov,* Tetiana Tkachenko and Vitalii Yevdokymenko



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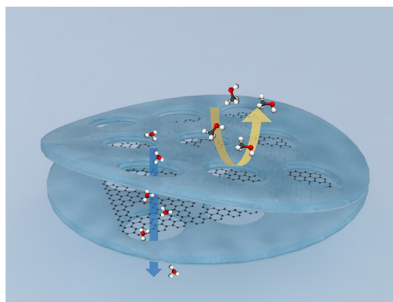
A first principles study on the stability and electronic and optical properties of 2D SbXY (X = Se/Te and Y = I/Br) Janus layers

A. E. Sudheer, Amrendra Kumar, G. Tejaswini, M. Vallinayagam, M. Posselt, M. Zschornak, C. Kamal and D. Murali*



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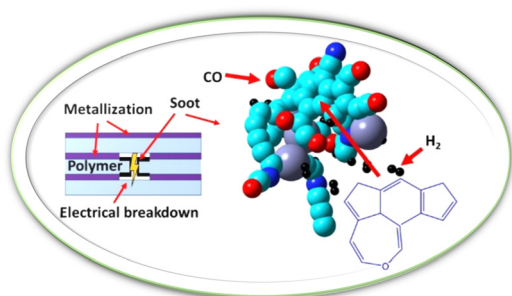
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Evaluation and optimization of polycarbonate track-etched (PCTE) membranes for direct methanol fuel cells

Zhixuan Ying, Yindong Wang, Wenjie Xi, Kejie Feng and Le Shi*

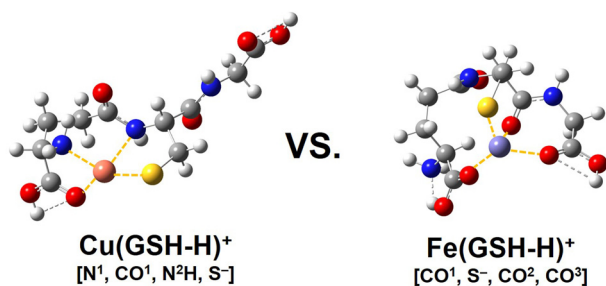
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Self-healing in dielectric capacitors: a universal method to computationally rate newly introduced energy storage designs

Nadezhda A. Andreeva* and Vitaly V. Chaban

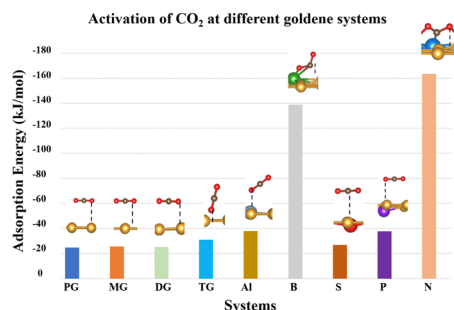
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Structural determination of Zn²⁺, Cu²⁺, and Fe²⁺ complexed with glutathione by IRMPD spectroscopy and complimentary *ab initio* calculations

Samantha K. Walker, Amanda R. Bubas, Brandon C. Stevenson, Evan H. Perez, Giel Berden, Jonathan Martens, Jos Oomens and P. B. Armentrout*

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Mechanistic insights into CO₂ activation on pristine, vacancy-containing and doped goldene: a single-atom layer of gold

Kamal Kumar, Nora H. de Leeuw, Jost Adam and Abhishek Kumar Mishra*

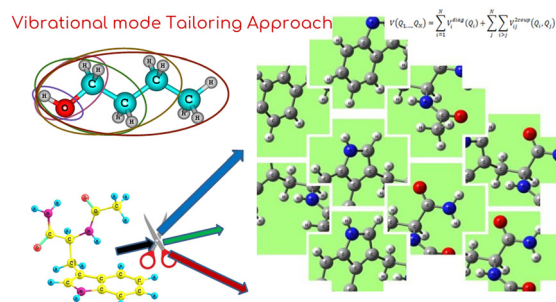


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Vibrational mode tailoring approach: an efficient route to compute anharmonic molecular vibrations of large molecules

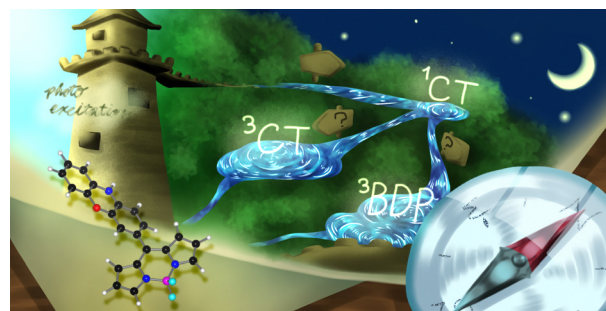
Hrishit Mitra, Dhiksha Sharma and Tapta Kanchan Roy*



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The molecular mechanism of the triplet state formation in bodipy-phenoxazine photosensitizer dyads confirmed by *ab initio* prediction of the spin polarization

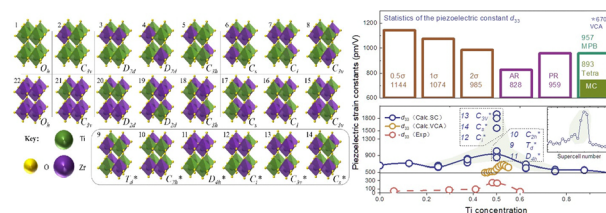
Maria Kosaka,* Katsuki Miyokawa and Yuki Kurashige*



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The local atomic distribution in tetragonal PZT

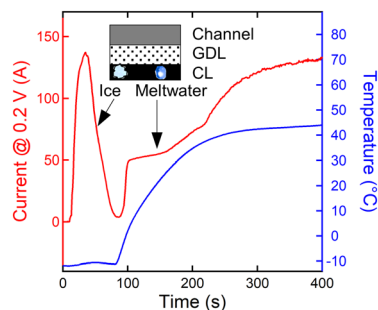
Junyu Niu, Chong Li and Zengzhe Xi*



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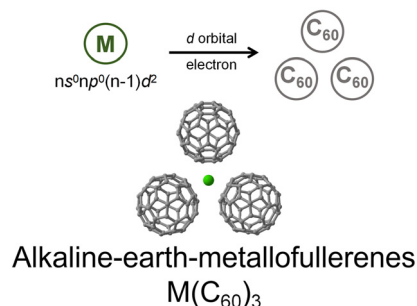
Neutron imaging for automotive polymer electrolyte fuel cells during rapid cold starts

Wataru Yoshimune,* Yuki Higuchi, Fangzhou Song, Shogo Hibi, Yoshihiro Matsumoto, Hirotochi Hayashida, Hiroshi Nozaki, Takenao Shinohara and Satoru Kato



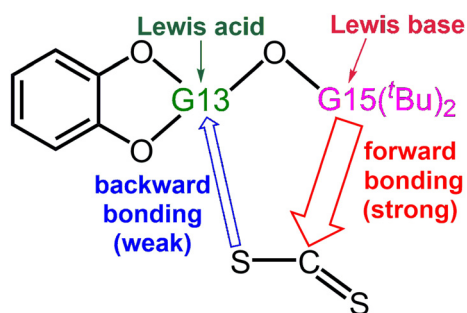
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20-electron exohedral alkaline-earth metallofullerenes $M(C_{60})_3$ ($M = Ca, Sr, \text{ and } Ba$)

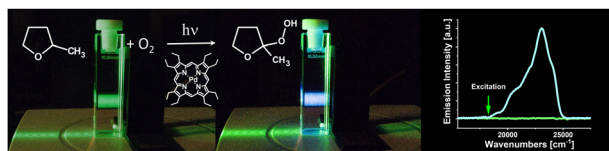
Feiyang Huang, Jian Zhou* and Tao Yang*

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Examining the reactivity of oxygen-bridged intramolecular group 13 element/phosphorus and boron/group 15 element frustrated Lewis pairs in 1,2-addition reactions with CS_2

Shi-Hao Wu and Ming-Der Su*

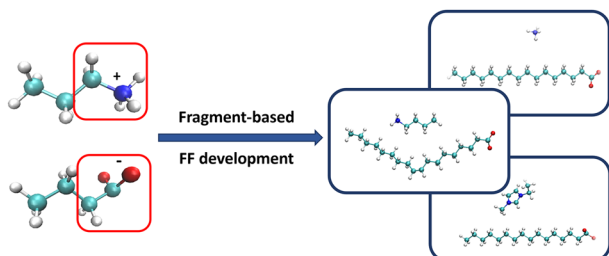
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Photoinduced removal of molecular oxygen from solutions

Barbara Golec, Natalia Dutkiewicz, Jakub Ostapko, Jacek Waluk and Aleksander Gorski*

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Investigating the properties of fatty acid-based ionic liquids: advancement in AMOEBA force field

Sahar Heidari and Hedieh Torabifard*

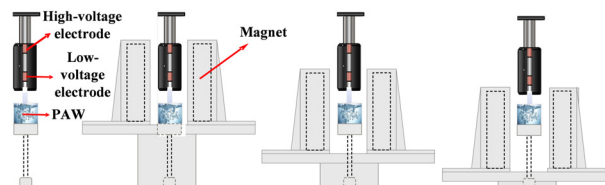


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Magnetic field enhanced discharge and water activation of atmospheric pressure plasma jet: effect of the assistance region and underlying physicochemical mechanism

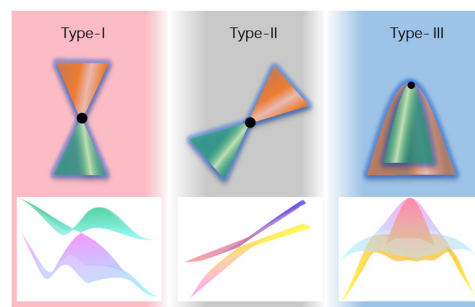
Xiong-Feng Zhou, Bin Chen, Hua Liao and Kun Liu*



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Multiple Weyl fermions and topological phase transition in two-dimensional ferromagnetic CrS₂

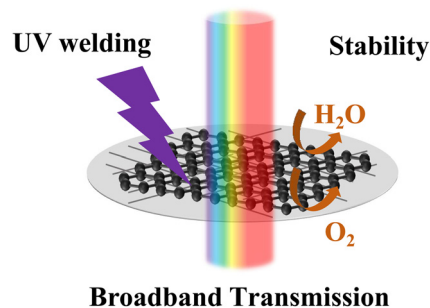
Shuo Zhang, Wenzhang Cheng, Lei Jin,* Ying Liu, Xuefang Dai, Guodong Liu and Xiaoming Zhang*



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A two-step junction welding technique for achieving high-performance broadband silver nanowire transparent conductive films

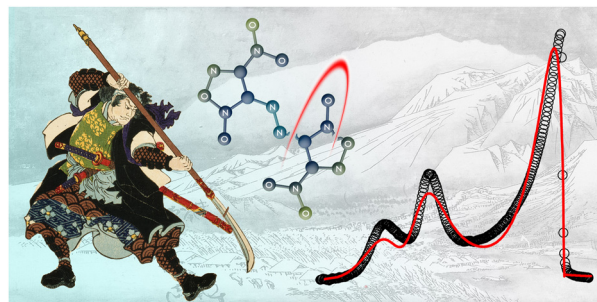
Shengyong Wang, Yongqiang Pan,* Shuai Wen, Jijie Zhao, Yuxuan Du, Fei Gao, Mengcong Li, Menglin Li and Huan Liu*



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Too fast and too furious: thermoanalytical and quantum chemical study of the thermal stability of 4,4'-dinitro-3,3'-diazonofuroxan

Vitaly G. Kiselev,* Artem R. Sadykov, Igor N. Melnikov, Igor V. Fomenkov, Leonid L. Fershtat, Alla N. Pivkina and Nikita V. Muravyev*



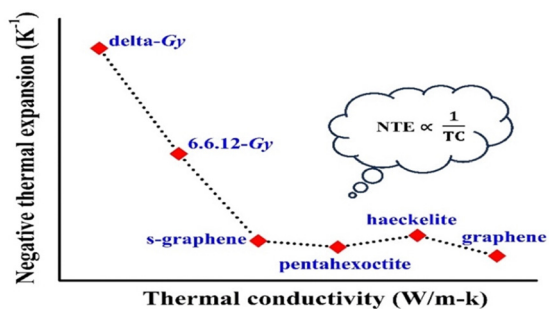
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Calculated ionization energies, orbital eigenvalues (HOMO), and related QSAR descriptors of organic molecules: a set of 61 experimental values enables elimination of systematic errors and provides realistic error estimates

Peter R. Tentscher

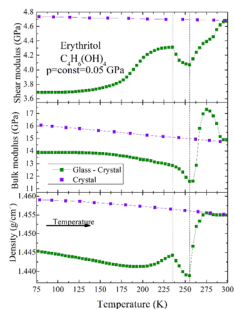
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Correlating negative thermal expansion and thermal conductivity in two-dimensional carbon-based materials

Soumya Mondal and Ayan Datta*

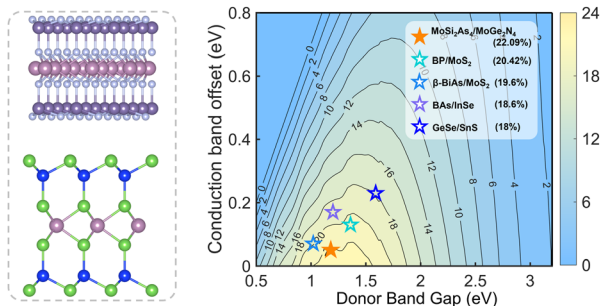
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Polyhydric alcohols under high pressure: comparative ultrasonic study of elastic properties

Elena L. Gromnitskaya,* Igor V. Danilov and Vadim V. Brazhkin

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Beyond 22% power conversion efficiency in type-II MoSi₂As₂/MoGe₂N₄ photovoltaic vdW heterostructure

Jing-yi Zhang, Xiao-bin Wu* and Jun-jie Shi

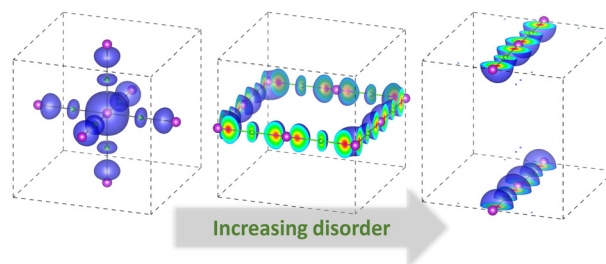


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Tuning the electronic dimensionality and bandgap in $\text{Cs}_2\text{AgBiX}_6$ ($X = \text{Br}, \text{Cl}$) for photovoltaic applications: a DFT-1/2 study of cation disorder

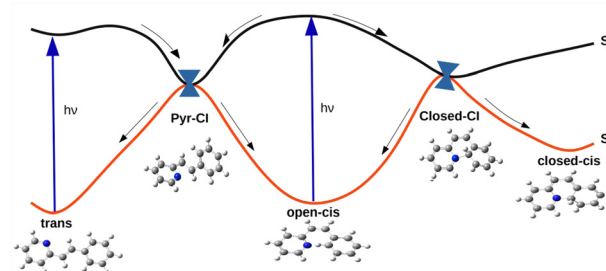
Vinut R. Vadagavi, R. Imran Jafri, Krishnakumar S. R. Menon and Suman Mandal*



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An *ab initio* study on the photoisomerization in 2-styrylpyridine

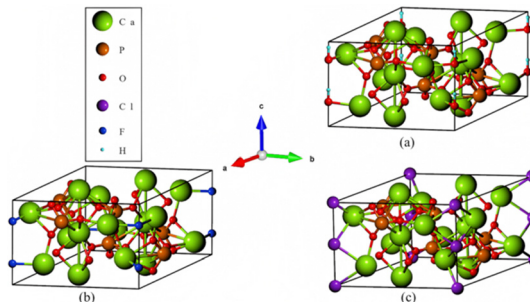
Derreck W. Nongspung and Aditya N. Panda*



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Benchmarking DFT approximations for studying apatites

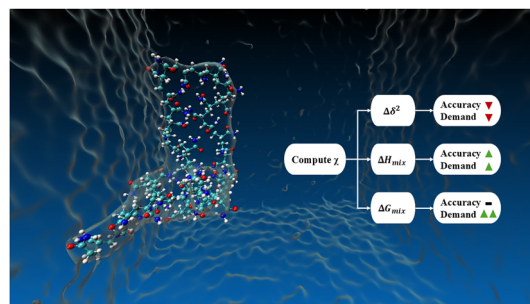
Aritri Roy, Bikash Kanungo, Puneet Kumar Patra* and Baidurya Bhattacharya



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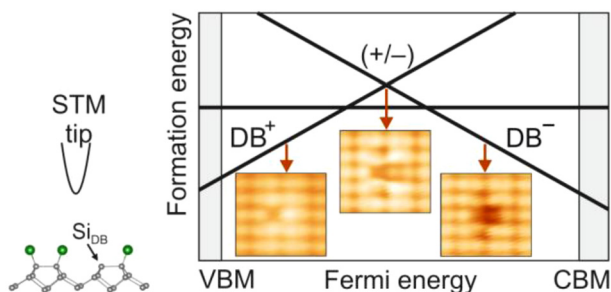
Solubility of selected polymers in cyclohexane: comparison between Flory–Huggins interaction parameters calculated using three different molecular dynamics simulation approaches

Gabriel P. Costa, Stanislav R. Stoyanov,* Qi Liu and Phillip Choi*



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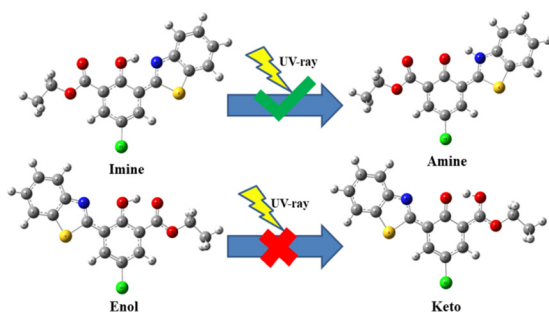
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Transitions between positive and negative charge states of dangling bonds on a halogenated Si(100) surface

Tatiana V. Pavlova* and Vladimir M. Shevlyuga

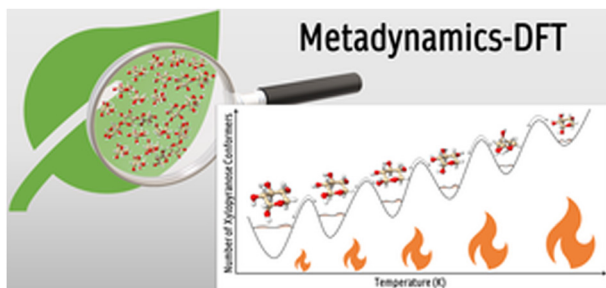
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Preference for excited state imine-amine isomerisation over enol-keto isomerisation: spectroscopic exploration and quantum chemical calculations

Souvik Santra, Rintu Mondal, Atanu Panja and Nikhil Guchhait*

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Ab initio conformational analysis of α/β -D-xylopyranose at pyrolysis conditions

Bernardo Ballotta,* Jacopo Lupi, Leandro Ayarde-Henriquez and Stephen Dooley

