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

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

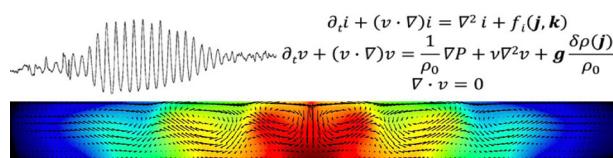


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Transport-driven chemical oscillations: a review

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

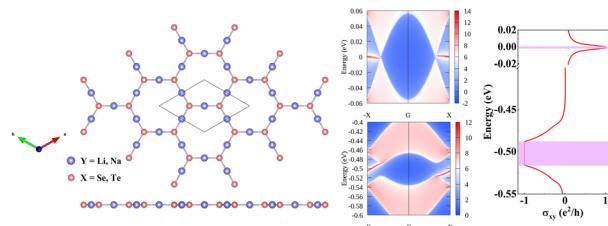


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The quantum anomalous Hall effect and strong robustness in two-dimensional p-state Dirac half-metals Y_3X_2 ($Y = \text{Li, Na}$; $X = \text{Se, Te}$)

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

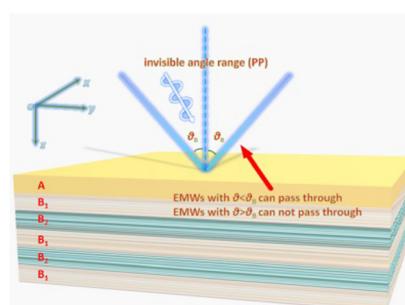


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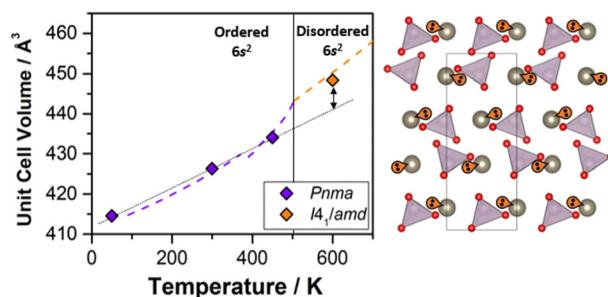
Hao-Ran Xu, Bao-Fei Wan and Hai-Feng Zhang*



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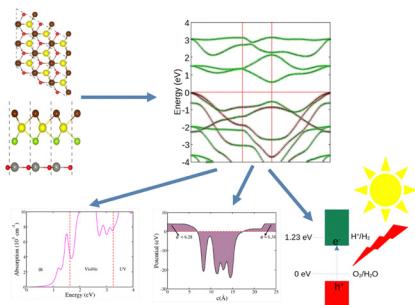
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Bryce G. Mullens, Frederick P. Marlton,* Matilde Saura-Múzquiz, Michelle Everett, Cheng Li, Alicia M. Manjon-Sanz, Matthew G. Tucker, Frederic Poineau, James Louis-Jean, Supratik Mukherjee, Subrata Mondal, Ganapathy Vaitheeswaran* and Brendan J. Kennedy



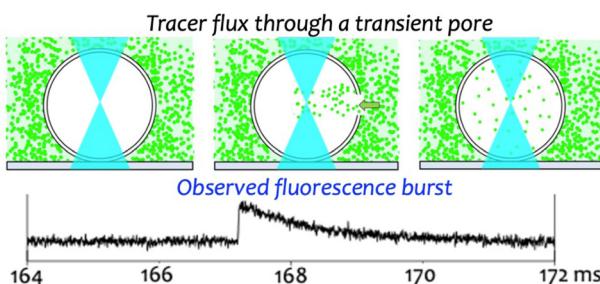
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**First principles study of photocatalytic activity in ZnO-Janus van der Waals heterostructures**

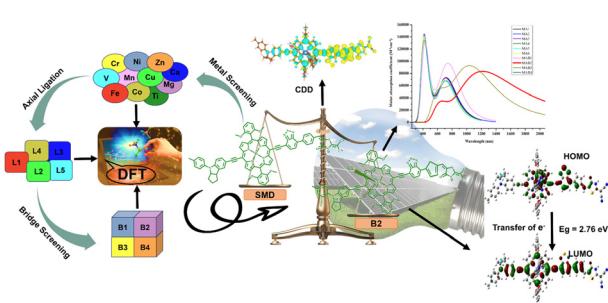
Tahir Wahab,* Antonio Cammarata* and Tomas Polcar

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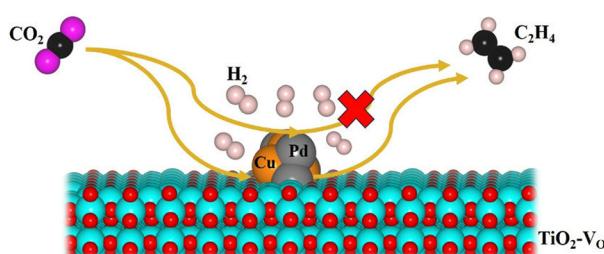
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Sajjad Hussain, Lina Zhang, Zhengzheng Xie,* Jianjun Yang and Qiuye Li*

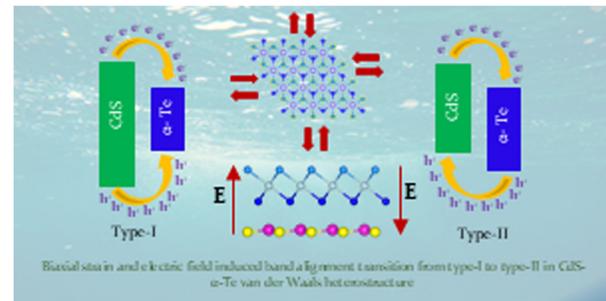


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Band alignment in CdS– α -Te van der Waals heterostructures for photocatalytic applications: influence of biaxial strain and electric field

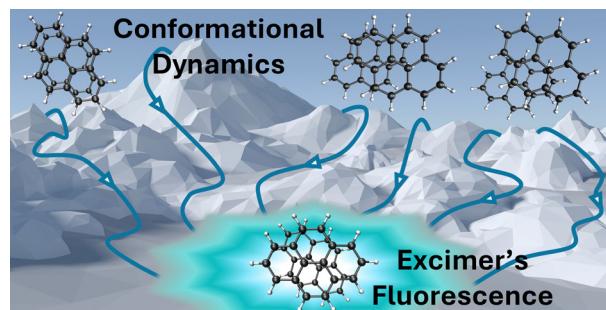
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Conformational dynamics of the pyrene excimer

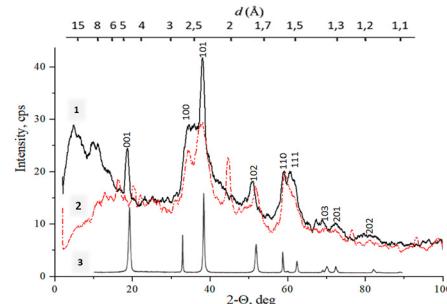
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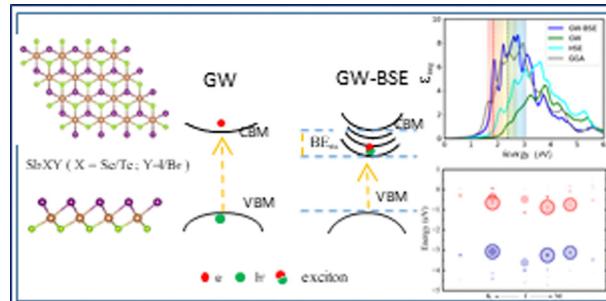
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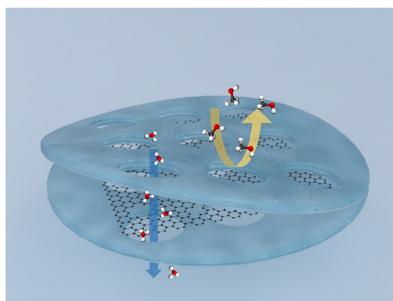
A first principles study on the stability and electronic and optical properties of 2D SbXY (X = Se/Te and Y = I/Br) Janus layers

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



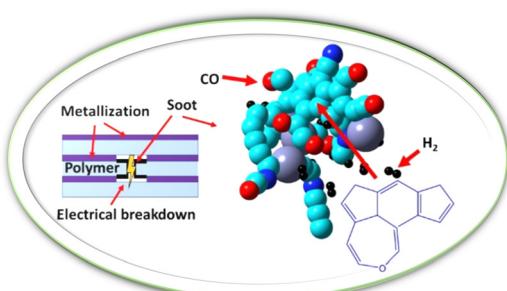
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Evaluation and optimization of polycarbonate track-etched (PCTE) membranes for direct methanol fuel cells

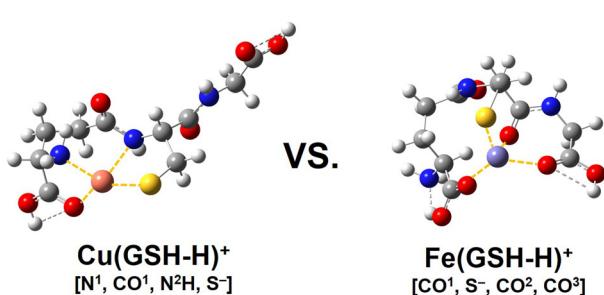
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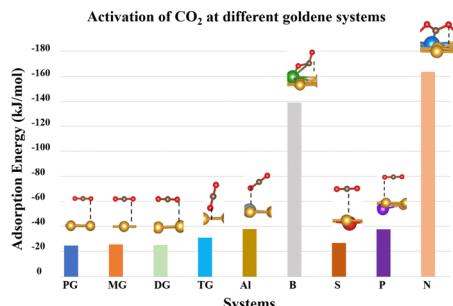
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Mechanistic insights into CO₂ activation on pristine, vacancy-containing and doped goldene: a single-atom layer of gold

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

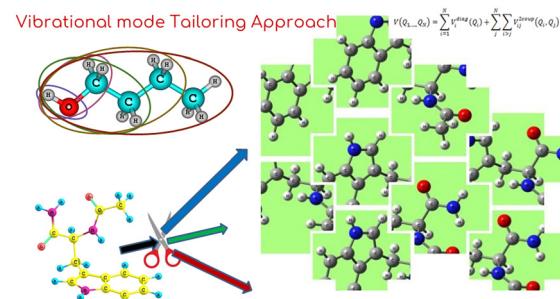


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Vibrational mode tailoring approach: an efficient route to compute anharmonic molecular vibrations of large molecules

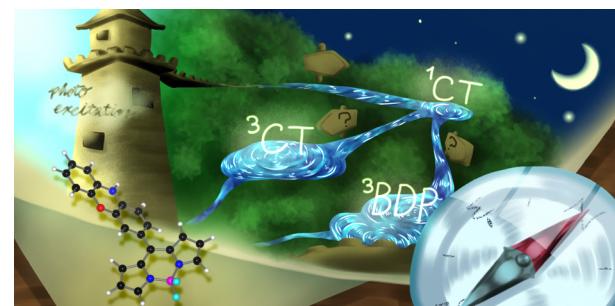
Hrishit Mitra, Dhiksha Sharma and Tapta Kanchan Roy*



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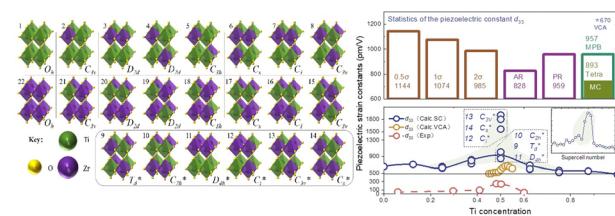
Maria Kosaka,* Katsuki Miyokawa and Yuki Kurashige*



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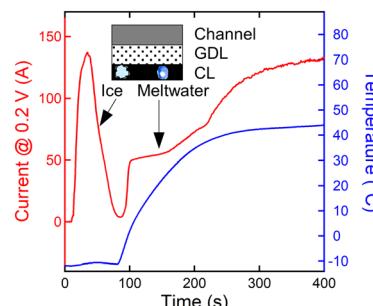
Junyu Niu, Chong Li and Zengzhe Xi*



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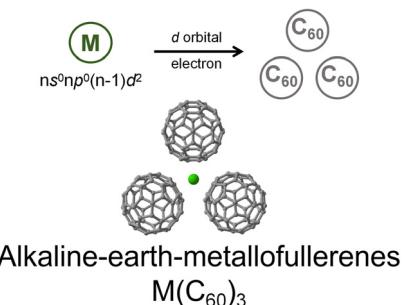
Neutron imaging for automotive polymer electrolyte fuel cells during rapid cold starts

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



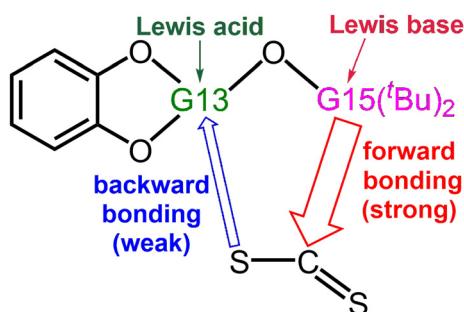
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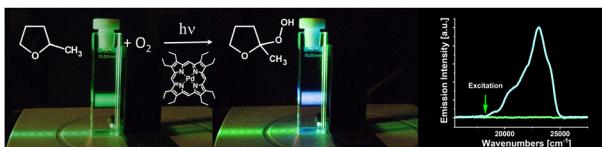
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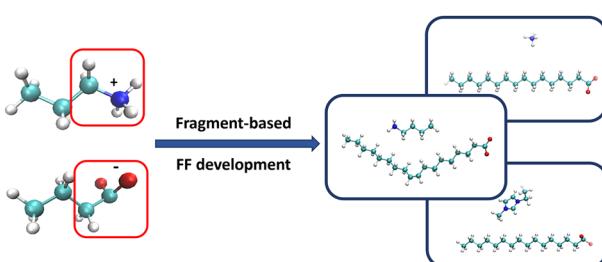
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Sahar Heidari and Hedieh Torabifard*

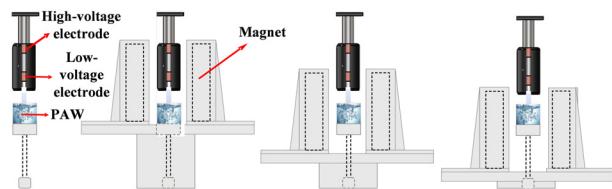


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Magnetic field enhanced discharge and water activation of atmospheric pressure plasma jet: effect of the assistance region and underlying physicochemical mechanism

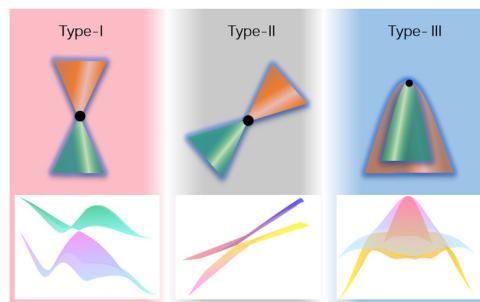
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Multiple Weyl fermions and topological phase transition in two-dimensional ferromagnetic CrS₂

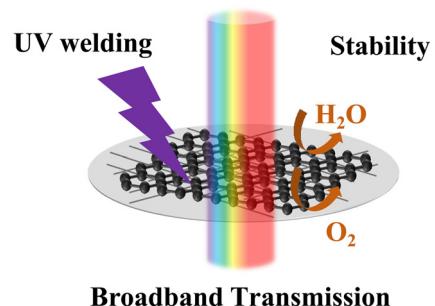
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A two-step junction welding technique for achieving high-performance broadband silver nanowire transparent conductive films

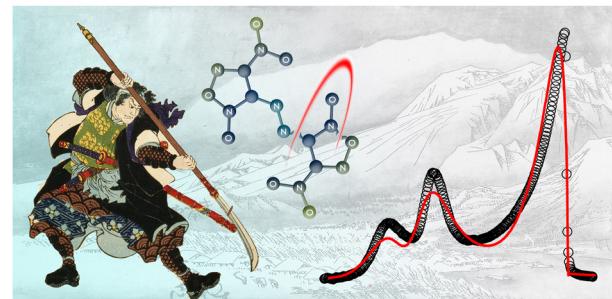
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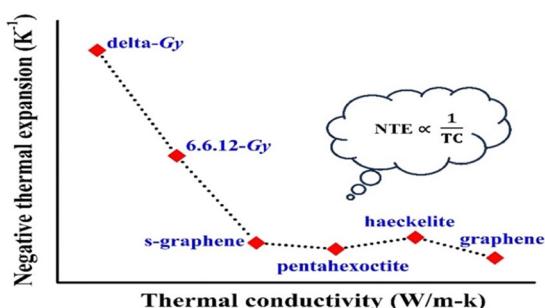
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Calculated ionization energies, orbital eigenvalues (HOMO), and related QSAR descriptors of organic molecules: a set of 61 experimental values enables elimination of systematic errors and provides realistic error estimates

Peter R. Tentscher

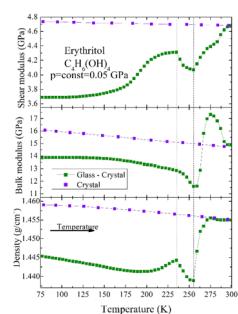
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Correlating negative thermal expansion and thermal conductivity in two-dimensional carbon-based materials

Soumya Mondal and Ayan Datta*

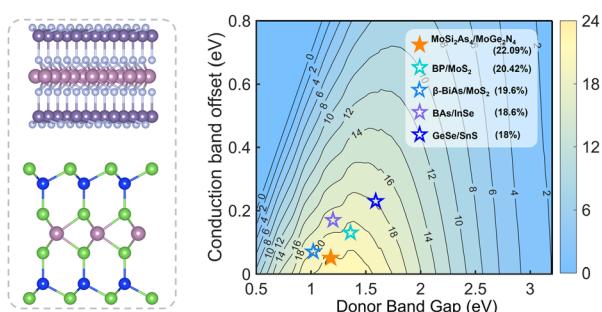
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Elena L. Gromnitskaya,* Igor V. Danilov and Vadim V. Brazhkin

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Beyond 22% power conversion efficiency in type-II MoSi₂As₄/MoGe₂N₄ photovoltaic vdW heterostructure

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

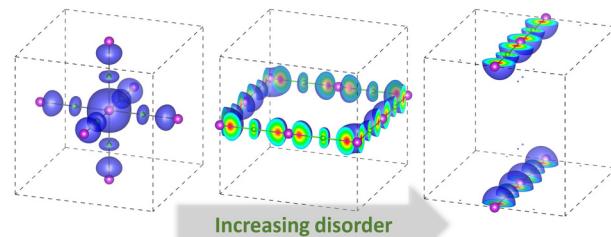


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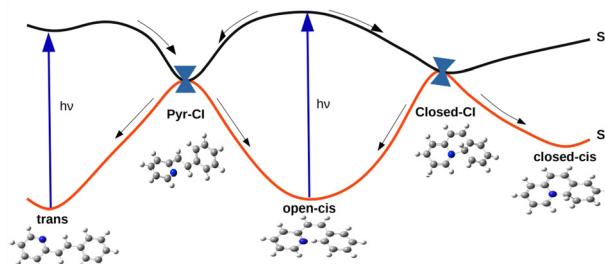
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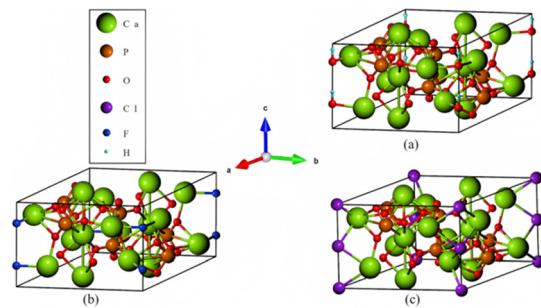
Derrick W. Nongspung and Aditya N. Panda*



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Benchmarking DFT approximations for studying apatites

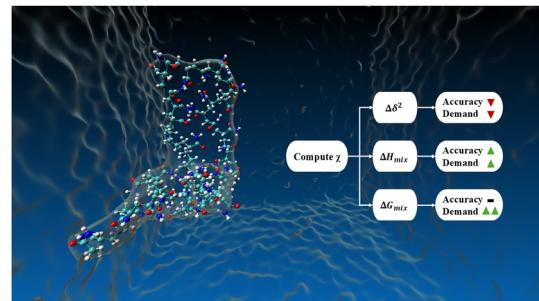
Aritri Roy, Bikash Kanungo, Puneet Kumar Patra* and Baidurya Bhattacharya



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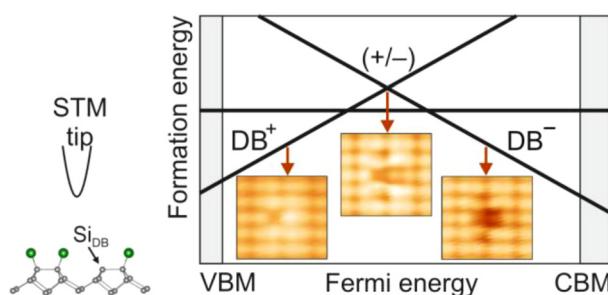
Solubility of selected polymers in cyclohexane: comparison between Flory–Huggins interaction parameters calculated using three different molecular dynamics simulation approaches

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



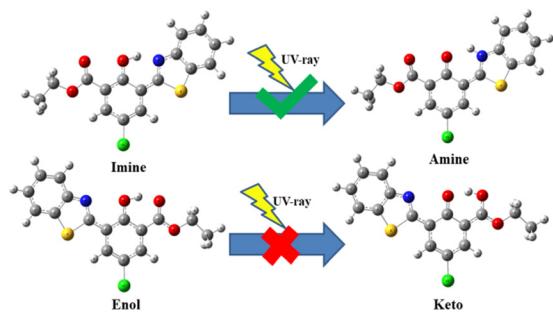
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**Transitions between positive and negative charge states of dangling bonds on a halogenated Si(100) surface**

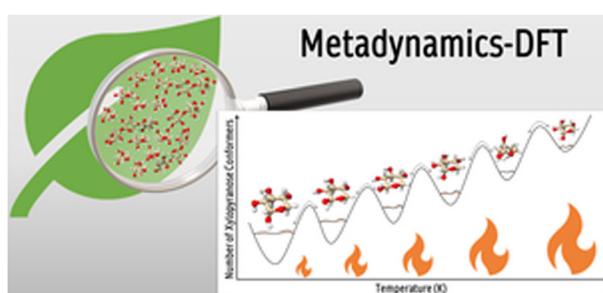
Tatiana V. Pavlova* and Vladimir M. Shevlyuga

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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

