

IN THIS ISSUE

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Cover

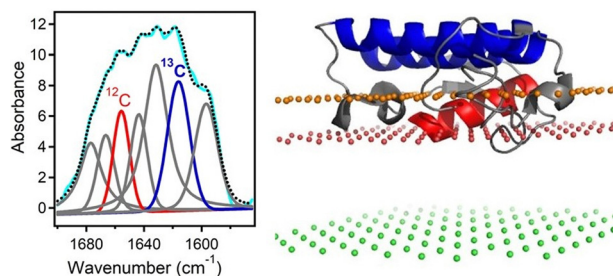
See Hannu Häkkinen
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Phys. Chem. Chem. Phys.,
2024, 26, 21954.

TUTORIAL REVIEW

21930

Analysis of protein–protein and protein–membrane interactions by isotope-edited infrared spectroscopy

Suren A. Tatulian

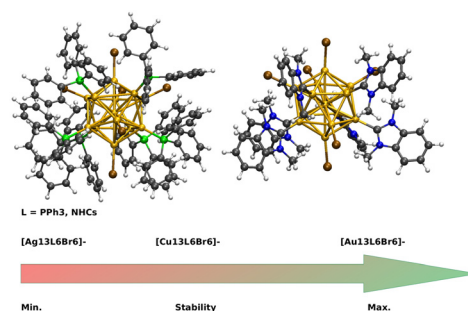


RESEARCH PAPERS

21954

Metal–ligand bond in group-11 complexes and nanoclusters

Maryam Sabooni Asre Hazer, Sami Malola and
Hannu Häkkinen*



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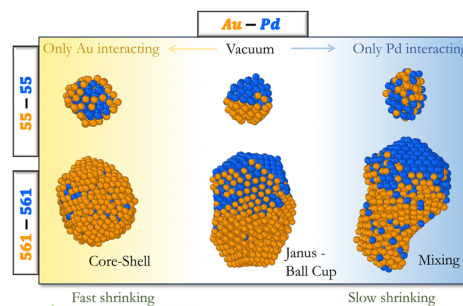


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21965

Coalescence of AuPd nanoalloys in implicit environments

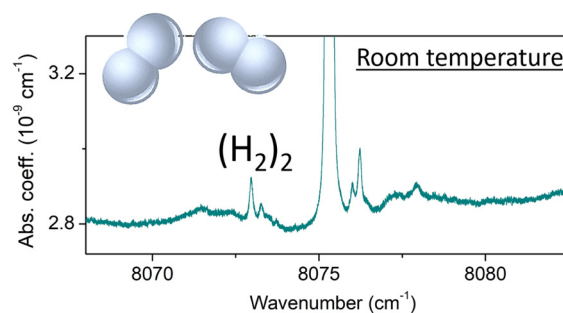
Sofia Zinzani and Francesca Baletto*



21974

Room temperature detection of the $(H_2)_2$ dimer

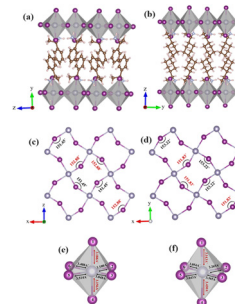
H. Fleurbaey, S. Kassi and A. Campargue*



21982

Unraveling the influence of organic cations on tuning electronic structures and spin-splitting in two-dimensional layered organic–inorganic tin-iodine perovskites

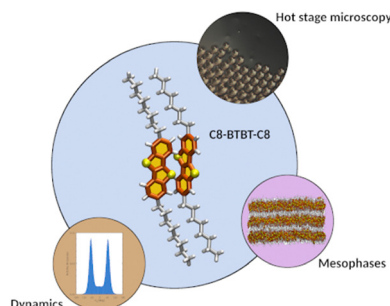
Abdesslem Jedidi,* Shatha M. Alamri, Norah O. Alotaibi, Souraya Goumri-Said* and Mohammed Benali Kanoun*



21990

Exploring the phase behavior of C8-BTBT-C8 at ambient and high temperatures: insights and challenges from molecular dynamics simulations

Mosè Casalegno,* Simone Provenzano, Guido Raos and Massimo Moret*





B. V. Padlyak, I. I. Kindrat,* V. T. Adamiv, A. Drzewiecki,
B. Cieniek and I. Stefaniuk

Pre-resonance enhancement in deep UV Raman spectra probes H-bonding properties of water

Pre-resonance effects in deep UV Raman spectra of normal and deuterated water

B. Rossi, M. Tommasini, P. M. Ossi* and M. Paolantoni

Electronic properties of pristine and doped graphitic germanium carbide nanomeshes

Sarah Gamal, M. Nashaat, Lobna M. Salah,
Nageh K. Allam and Ahmed A. Maarouf*

Kinetics of the mechanically induced ibuprofen–nicotinamide co-crystal formation by *in situ* X-ray diffraction

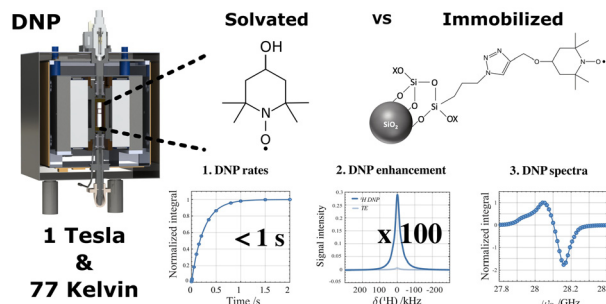
Lucia Casali, Maria Carta, Adam A. L. Michalchuk,
Francesco Deloqui* and Franziska Emmerling*

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Full optimization of dynamic nuclear polarization on a 1 tesla benchtop polarizer with hyperpolarizing solids

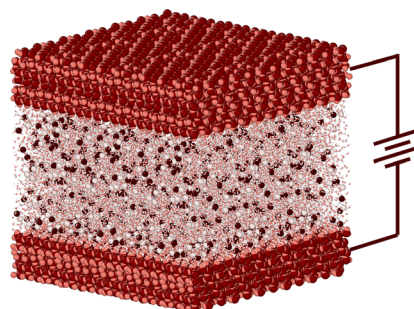
Ewoud Vaneeckhaute,* Charlotte Bocquelet, Léa Bellier, Huu-Nghia Le, Nathan Rougier, Shebha Anandhi Jegadeesan, Sanjay Vinod-Kumar, Guinevere Mathies, Laurent Veyre, Chloe Thieuleux, Roberto Melzi, Daniel Banks, James Kempf, Quentin Stern and Sami Jannin



22062

Water and ions in electrified silica nano-pores: a molecular dynamics study

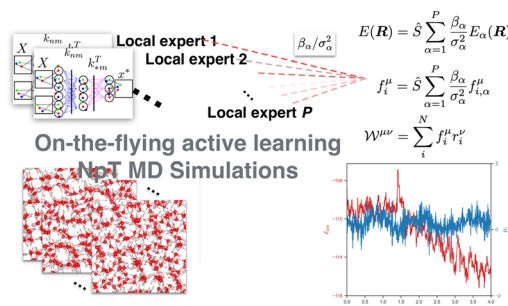
Mahdi Tavakol* and Kislou Voitchovsky*



22073

Active sparse Bayesian committee machine potential for isothermal–isobaric molecular dynamics simulations

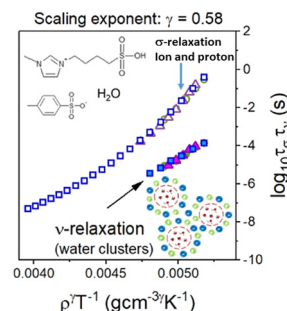
SooHaeng Yoo Willow, Dong Geon Kim, R. Sundheep, Amir Hajibabaei, Kwang S. Kim and Chang Woo Myung*



22083

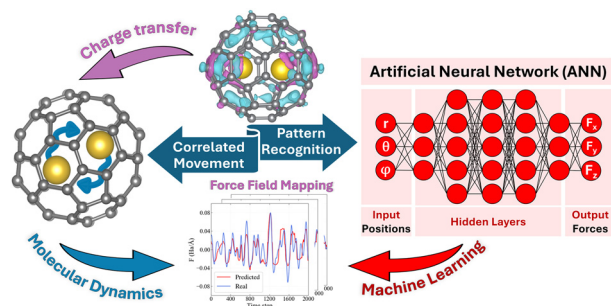
Origin of ρ^{γ}/T scaling of primary and secondary conductivity relaxation times in mixture of water with protic ionic liquid

K. L. Ngai



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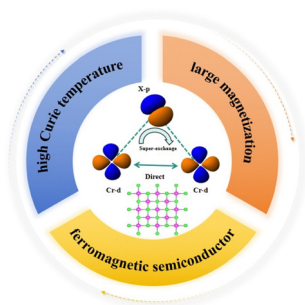
22090



Collective dynamics of Ca atoms encapsulated in C₆₀ endohedral fullerenes

Mihaela Cosinschi, Amanda T. Preda, C.-A. Pantis-Simut, N. Filipoiu, I. Ghitui, M. A. Dulea, L. Ion, A. Manolescu and G. A. Nemnes*

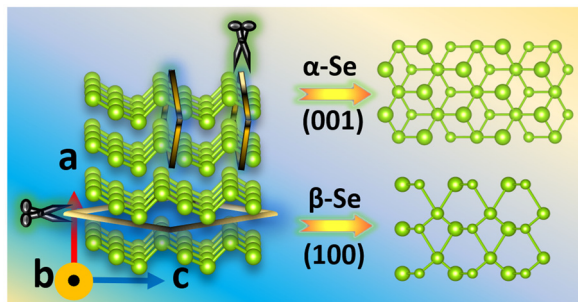
22099



Two-dimensional ferromagnetic semiconductor Cr₂XP: first-principles calculations and Monte Carlo simulations

Xiao-Ping Wei,* Lan-Lan Du, Jiang-Liu Meng and Xiaoma Tao

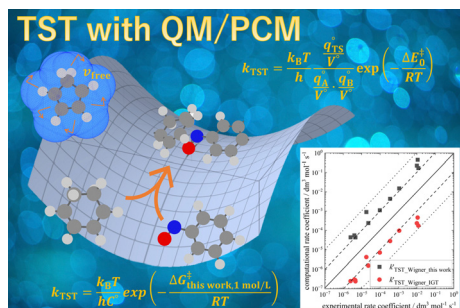
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Multivalency-induced structural variations of 2D selenium nanosheets: facile solution-phase synthesis and optical properties

Swathi V. M., Arjun K., Anju Rajan, Raghu Chathanathodi, Karthikeyan Balasubramanian and Aji A. Anappara*

22122



Computation of rate coefficients in solutions based on transition state theory combined with a heuristically corrected polarizable continuum model: intermolecular Diels–Alder reactions as case studies

Yu-ichiro Izato,* Mitsuo Koshi and Atsumi Miyake

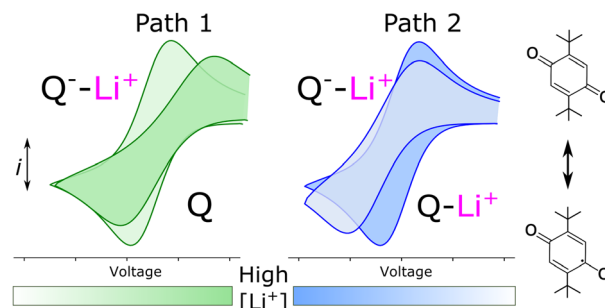


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22134

The effect of ionic association on the electrochemistry of redox mediators for Li–O₂ batteries: developing a theoretical framework

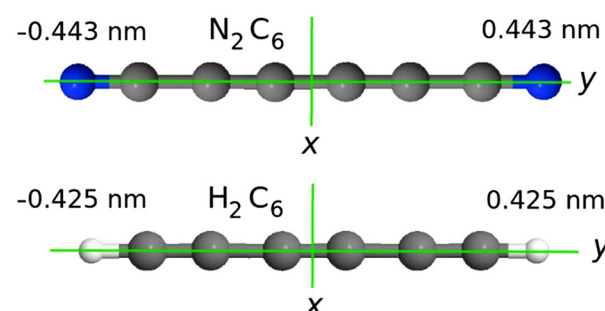
Gabriela Horwitz, Vera Kunz, Samuel P. Niblett and Clare P. Grey*



22149

Electronic structure, absorption spectra and oxidation dynamics in polyynes and dicyanopolyynes

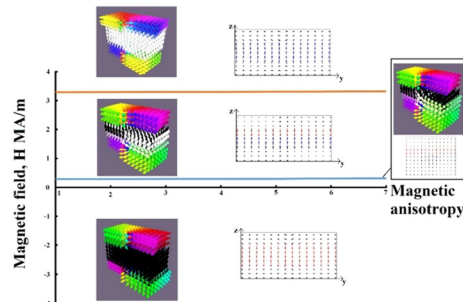
Lazaros Chalkopiadis, Konstantinos Lambropoulos and Constantinos Simserides*



22164

Magnetoelectric effects in magnetic films with alternating magnetic anisotropy: the emergence and stability of Bloch points

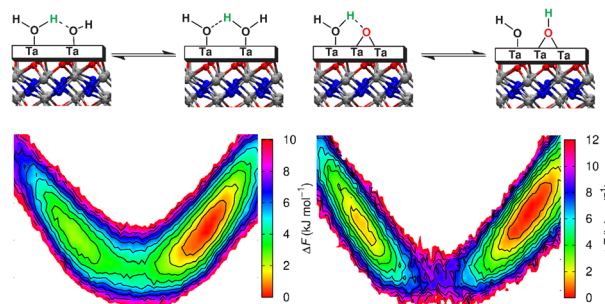
Zukhra Gareeva,* Viktoria Filippova, Nikolai Shulga and Rurik Doroshenko



22173

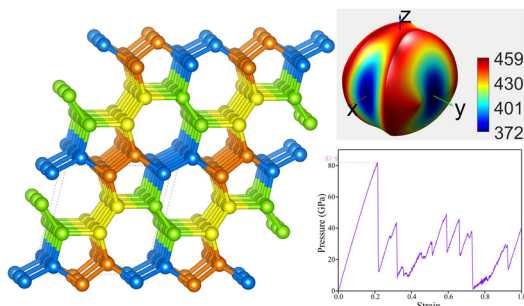
Molecular insights into the water dissociation and proton dynamics at the β-TaON (100)/water interface

Sagarmoy Mandal and Tushar Kanti Ghosh*



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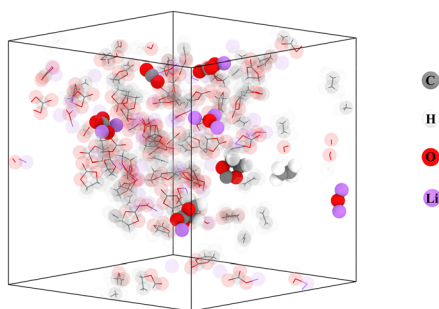
22182



A novel sp^3 carbon allotrope with 4+5+6+7+8 odd-even ring

Tao Yu, Sheng-Cai Zhu* and Yanglong Hou*

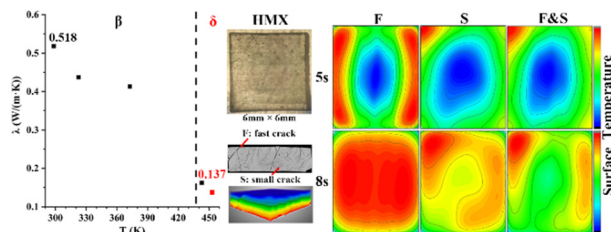
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Comparative study of the reductive decomposition reaction of ethylene carbonate in lithium battery electrolyte: a ReaxFF molecular dynamics study

Jingqi Gao, Ruitian He and Kai H. Luo*

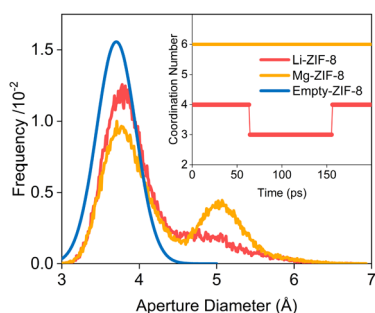
22208



Research on the mechanism of threefold discrepancy in thermal conductivity between room temperature and phase transition temperature for 1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) crystals

He Wang, Wentao Liang, Xiangqi Wang, Hao Wang, Di Mai, Cheng Zhong, Xiaoyu Sun, Rucheng Dai, Zhongping Wang, Xianxu Zheng,* Wanguo Zheng* and Zengming Zhang*

22220



The mechanisms underlying Li^+/Mg^{2+} separation in ZIF-8 under an electric field from atomistic simulations

Xiang-Long Fu, Fan Zheng, Shi-Jie Xie,* Yan-Li Ji* and Cong-Jie Gao

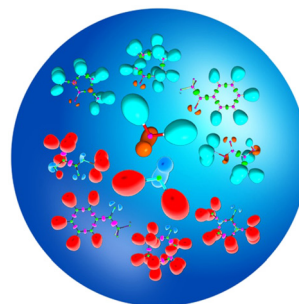


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Probing microhydration-induced effects on carbonyl compounds

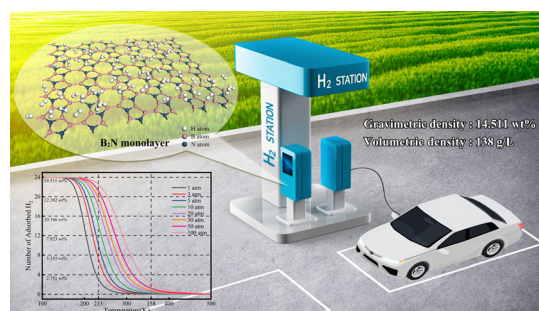
Olivier Aroule, Mahmoud Jarraya, Emilie-Laure Zins* and Majdi Hochlaf*



22240

Reversible hydrogen storage and release mechanism of a B₂N monolayer: a first-principles insight

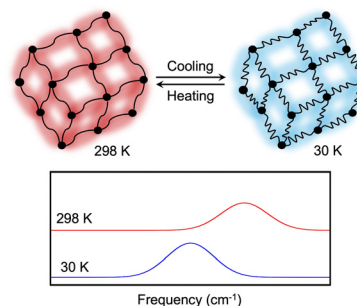
Zonggang Qiu, Jiyuan Guo,* Qun Wang, Han Wang and Xiangxiang Tan



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Temperature-dependent structural dynamics in covalent organic frameworks observed by cryogenic infrared spectroscopy

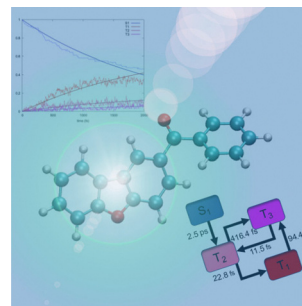
Silas O. Frimpong, Nathan McLane, Matthew Dietrich, Garrison A. Bauer, Michael R. Baptiste, Leah G. Dodson* and Mercedes K. Taylor*



22261

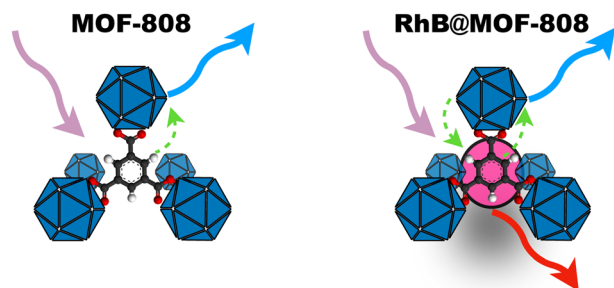
Intersystem crossing in a dibenzofuran-based room temperature phosphorescent luminophore investigated by non-adiabatic dynamics

Pelin Ulukan, Elise Lognon,* Saron Catak and Antonio Monari*



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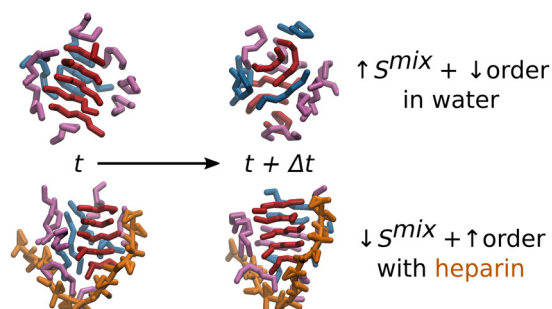
22269



Unveiling MOF-808 photocycle and its interaction with luminescent guests

G. Ficarra, A. Sciortino,* L. G. Barbata, R. Ettlinger, V. De Michele, E. Marin, M. Cannas, R. E. Morris and G. Buscarino*

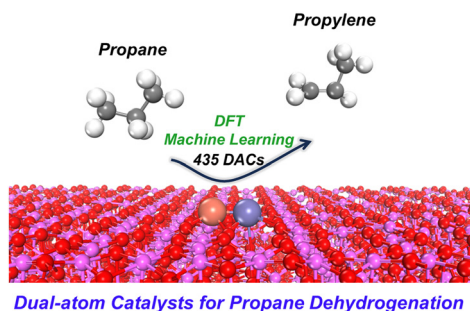
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Unravelling heparin's enhancement of amyloid aggregation in a model peptide system

Suhas Gotla, Anushka Poddar, Ilana Borison and Silvina Matysiak*

22286



Discovery of highly efficient dual-atom catalysts for propane dehydrogenation assisted by machine learning

Xianpeng Wang, Yanxia Ma, Youyong Li, Lu Wang* and Lifeng Chi*

CORRECTIONS

22292

Correction: First-principles calculations of interfacial thermal transport properties between SiC/Si substrates and compounds of boron with selected group V elements

Zhehao Sun, Kunpeng Yuan, Xiaoliang Zhang* and Dawei Tang*



CORRECTIONS

22293

Correction: Exploring the properties of $\text{Zr}_2\text{CO}_2/\text{GaS}$ van der Waals heterostructures for optoelectronic applications

Altaf Ur Rahman,* Muhammad Abdul,* Altaf Karim, Gul Rahman,* Islam H. El Azab and Bao Jingfu

