

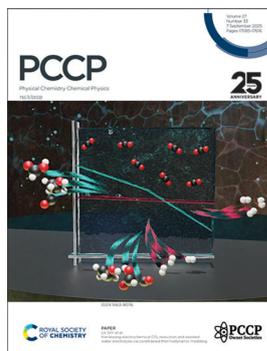
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ISSN 1463–9076 CODEN PPCPFQ 27(33) 17085–17616 (2025)



Cover

See Reum N. Scott, Phillip J. Milner, Julia Dshemuchadse, pp. 17183–17197. Image reproduced by permission of Reum N. Scott, Phillip J. Milner and Julia Dshemuchadse from *Phys. Chem. Chem. Phys.*, 2025, 27, 17183.



Inside cover

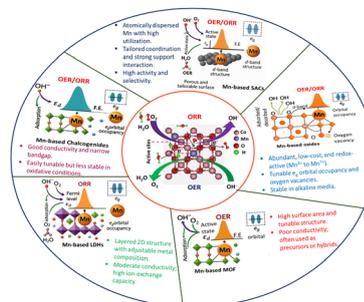
See Uk Sim *et al.*, pp. 17198–17211. Image reproduced by permission of Uk Sim from *Phys. Chem. Chem. Phys.*, 2025, 27, 17198.

REVIEWS

17099

Mn-based noble metal-free electrocatalysts: advancing the OER and the ORR through innovation and future insights

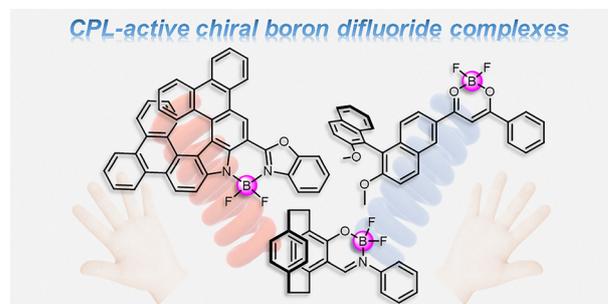
Anup Bist and Sungjin Park*



17116

Recent advances in circularly polarized luminescence (CPL) of chiral boron difluoride complexes

Masahiro Ikeshita* and Takashi Tsuno*



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Fundamental questions
Elemental answers

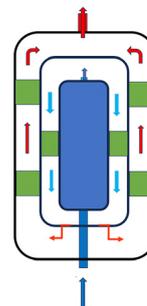


PERSPECTIVES

17130

Magneto-chemistry of catalysts for liquid hydrogen production and storage

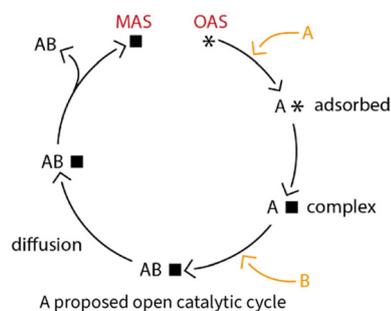
Ernest Ilisca



17157

Concepts and tools for integrating multiscale dynamics into reaction kinetics

Toyin Omojola*

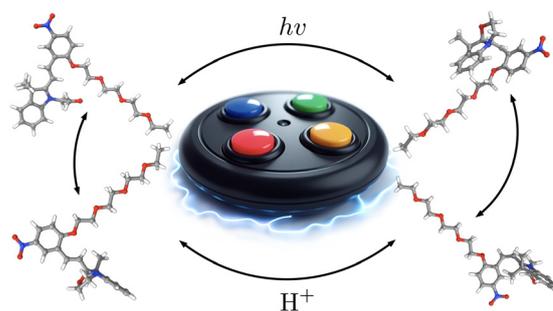


COMMUNICATION

17178

Substituent effects in a six-state molecular switch

Rachael Hannah, Kirsten M. van der Geest, Shahrzad Shafei, Ben L. Feringa and Ryan C. Chiechi*

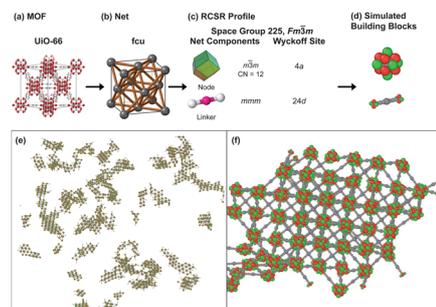


RESEARCH PAPERS

17183

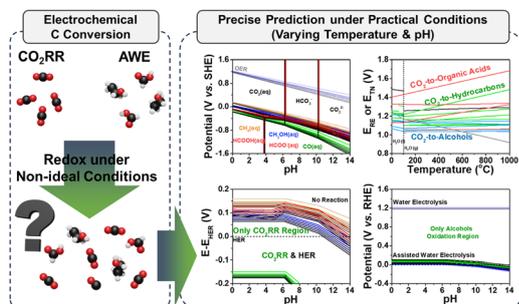
A coarse-grained simulation toolkit for metal–organic framework synthesis

Reum N. Scott,* Phillip J. Milner* and Julia Dshemuchadse*



RESEARCH PAPERS

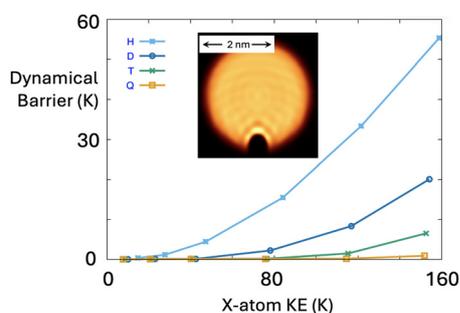
17198



Harnessing electrochemical CO₂ reduction and assisted water electrolysis *via* constrained thermodynamic modeling

Jinuk Choi, Hyojung Lim, Subramani Surendran, Seonghyeon Park, Junho Shim, Gyoung Hwa Jeong and Uk Sim*

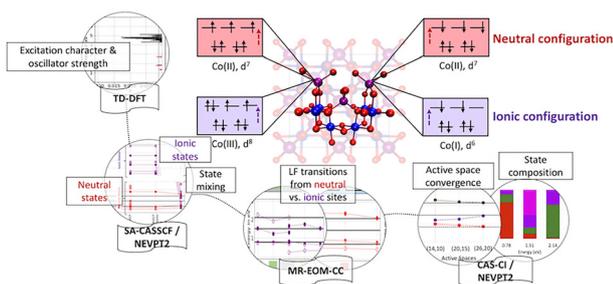
17212



Quantum dynamics of the temporary capture of light atoms by superfluid helium nanodroplets at very low collision energies ($\approx 1\text{--}13$ meV): the case of the hydrogen atom and its isotopes

Michael Sternberg, Stephen K. Gray and Miguel González*

17225



Revisiting the band gap problem in bulk Co₃O₄ and its isostructural Zn and Al derivatives through the lens of theoretical spectroscopy

Anneke Dittmer, Tiago Leyser da Costa Gouveia, Kantharuban Sivalingam, Serena DeBeer,* Frank Neese* and Dimitrios Maganas*

17245



Revisiting the bonding nature of pyramidane: an analogue of the CO molecule

Qinqin Yuan, Zhiruo Ding, Dan Li* and Longjiu Cheng*



17254

Contact angle determination as a function of solid–liquid molecular characteristics *via* the Kirkwood–Buff route

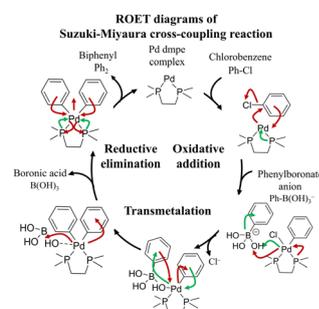
Patrick Tabeling

$$\cos \theta \approx 0.94 \frac{\rho_L^2 \Lambda}{\gamma}$$

17261

Tracking electron motion driving the Suzuki–Miyaura cross-coupling reaction

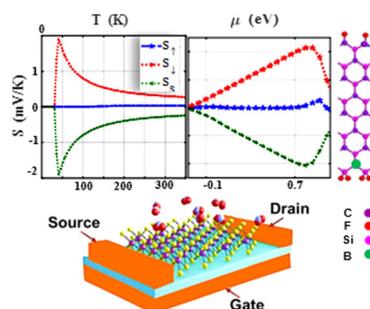
Noriyuki Takai, Takuro Tsutsumi, Tetsuya Taketsugu and Takao Tsuneda*



17270

Spin thermoelectric properties in fluorinated asymmetric zigzag SiC nanoribbons with boron and nitrogen impurities

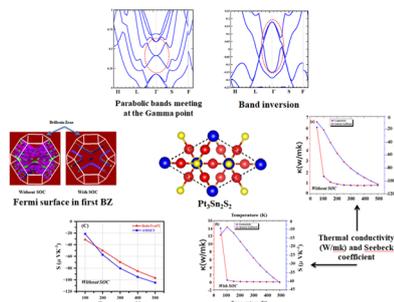
Somaye Esteki and Rouhollah Farghadan*



17280

Exploring the pressure and spin–orbit coupling effects in Pt₃Sn₂S₂: a kagome-type analog of Co₃Sn₂S₂

Ravi Trivedi, Seetha Lakshmy, Heera T. Nair, Alok Shukla, Medha Rakshit and Brahmananda Chakraborty*



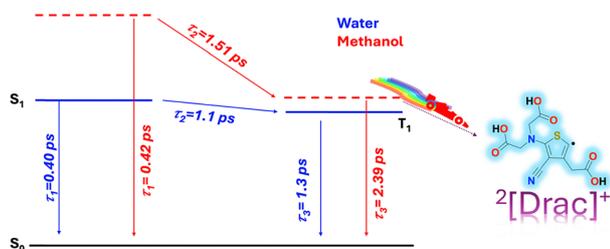
17291



Influence of hydration, hydroxylation, and doping of TiO₂(110) on the adsorption and decomposition of sarin: a density functional theory investigation

Yenny Cardona Quintero and Ramanathan Nagarajan*

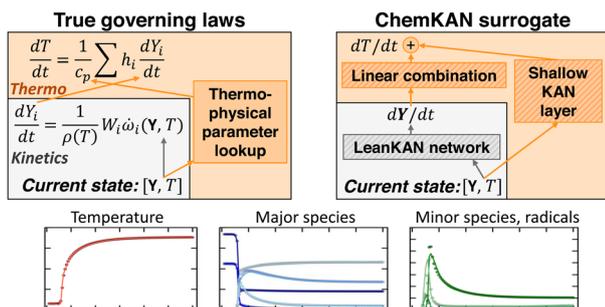
17303



Exploring radical formation and ultrafast intersystem crossing in a heavy-atom-free thiophene derivative

Luca M. Sihm,* Robert B. Vadell, Rafael B. Araujo, Atripan Mukherjee, Miroslav Kloz, Jacinto Sá and Henrique E. Toma

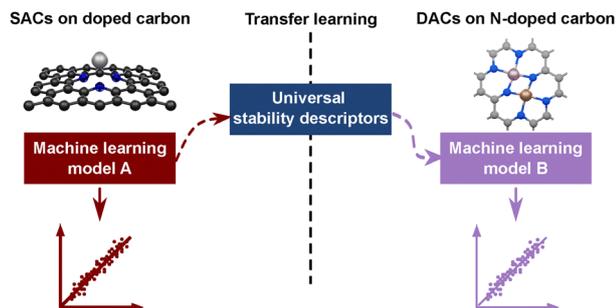
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ChemKANs for combustion chemistry modeling and acceleration

Benjamin C. Koenig, Suyong Kim and Sili Deng*

17331



Transfer learning with domain knowledge adaptation for stability evaluation of dual-atom catalysts on nitrogen-doped carbon

Maria G. Minotaki and Núria López*

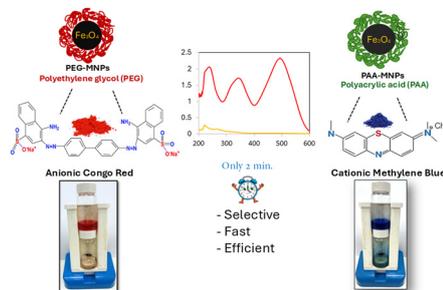


RESEARCH PAPERS

17341

Selective, effective, and rapid removal of cationic and anionic organic dyes using various tailored polymer-coated (PEG, PVP, PAA/starch) magnetite nanoparticles

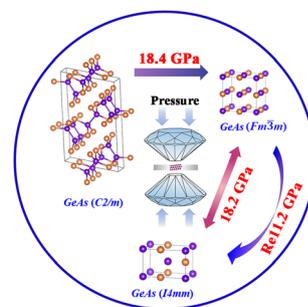
Hawra A. AlSabbagh, Kawthar M. AlDamestani, Wael A. Amer, Javed Iqbal, O. M. Lemine, Nawal Madkhali and Kheireddine El-Boubbou*



17360

Phase transition and in-plane anisotropy of GeAs under high pressure

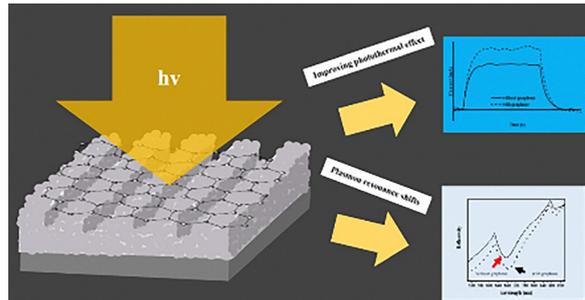
Junbo Wang, Zilong Zhang, Shiquan Feng, Haining Li, Xiang Zhu, Kun Yang* and Xuerui Cheng*



17368

Enhancement of the photothermal performance of silver nanoparticle grating films via graphene deposition

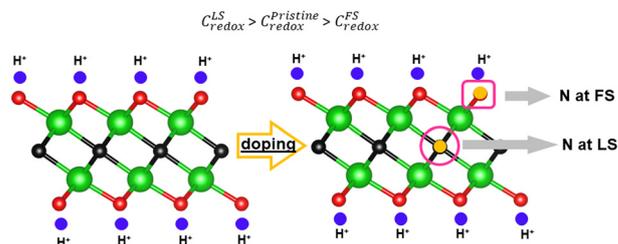
Siriporn Anuthum, Chutiparn Lertvachirapaiboon, Ryosuke Ishikawa, Sachiko Jonai, Kazunari Shinbo, Kontad Ounnunkad* and Akira Baba*



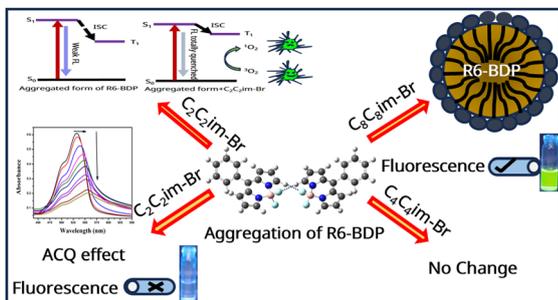
17376

First-principles investigation of nitrogen doping effects on the capacitance behavior of V₂CT_x MXenes

Sruthi T.,* Mandira Das and Vincent Mathew



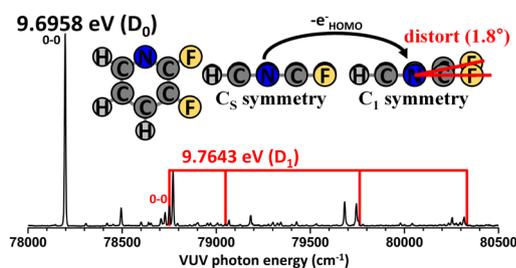
17384



Enhancement of the triplet photosensitizing ability of BODIPY dyes by controlled red-shifted H-aggregate formation using ionic liquids: insights from spectroscopy, microscopy, DFT and biological studies

Nayana Nupur Das, Soumyaditya Mula, Dhanya Rajendrababu, Sivan Velmathi* and Debashis Majhi*

17399

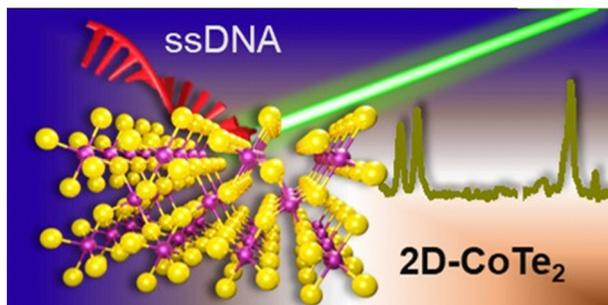


VUV-MATI spectroscopy and FC simulations reveal fluorine position-dependent ionization in 2,3-DFP, inducing a nonplanar D_0 and oblate D_1 cationic structure.

Fluorine position-dependent ionization dynamics and structural distortion in 2,3-difluoropyridine: a VUV-MATI and theoretical study

Hyojung Kim, Sung Man Park and Chan Ho Kwon*

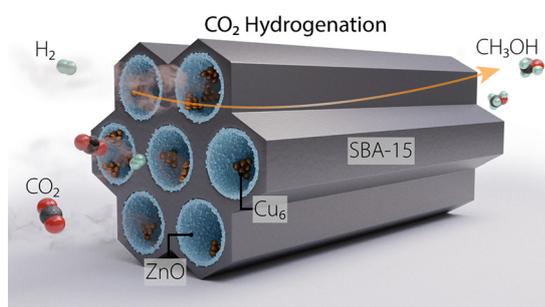
17407



Nucleobase identification using two-dimensional cobalt telluride

Anyesha Chakraborty, Anurag Upadhyaya, Solomon Demiss Negedu, Suman Sarkar, Basudev Lahiri, Prabal Kumar Maiti* and Chandra Sekhar Tiwary*

17420



CO₂ hydrogenation to methanol via ZnO-SBA-15-supported Cu₆ catalysts

Sara Mirzakhani, Angie F. J. Tan, Deborah Crittenden, Majid Masteri-Farahani and Alex C. K. Yip*

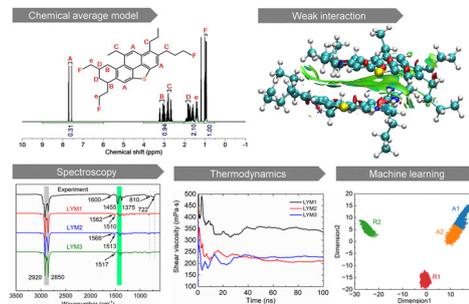


RESEARCH PAPERS

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New chemical average model for molecular simulations of the asphalt system

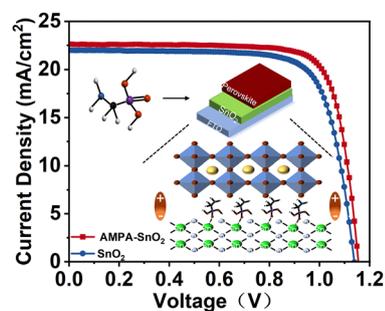
Zhengwu Long and Lingyun You*



17455

Dual-anchor interface engineering with a phosphonic acid modifier for improving perovskite solar cell performance

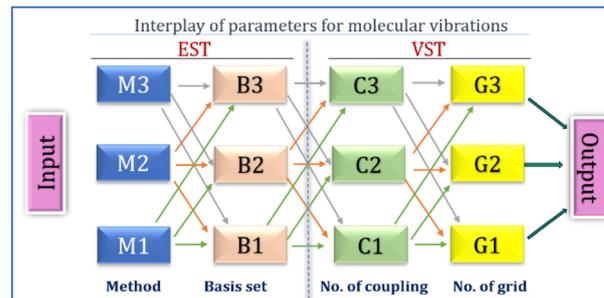
Wang Yao, Zijin Qiao, Zhirui Chen, Jiaqi Wang and Cheng Mu*



17464

Deciphering the interplay of different electronic and vibrational structure theory parameters for the computation of anharmonic molecular vibrations

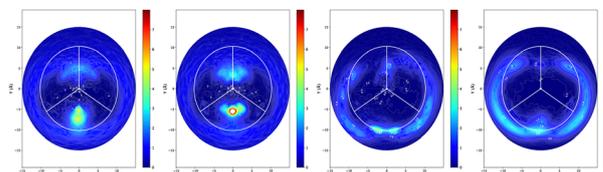
Dhiksha Sharma and Tapta Kanchan Roy*



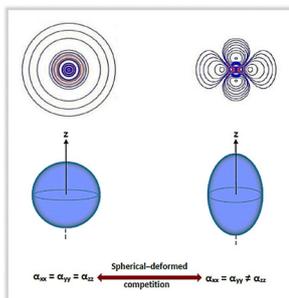
17481

Molecular dynamics studies of temperature-induced DNA-cation interaction: role of valency and size

Devendra Saini and Navin Singh*



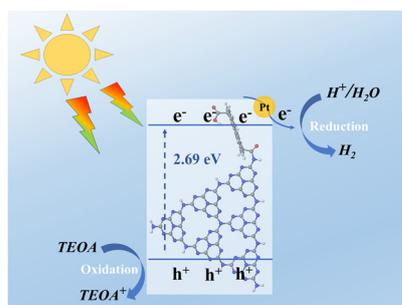
17492



Theoretical determination of linear and nonlinear optical properties as well as electric anisotropies of elements of the Periodic Table: a density functional theory study

Mahnaz Jabbarzadeh Sani

17504



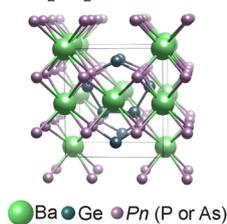
Regulating the exciton dissociation and charge carrier behavior of graphitic carbon nitride via 3,9-erylenedicarboxylic acid for efficient photocatalytic hydrogen evolution

Mingxiu Huang, Shiyi Fang, Linyue Xu, Huili Xie, Naseer Ahmad, Wei Sun and Bei Wang*

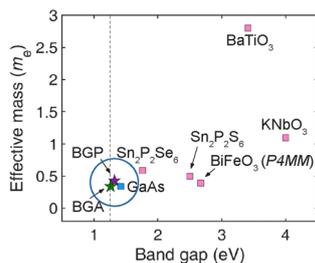
17514

Promising ferroelectric materials

BaGe_2Pn_2 ($\text{Pn} = \text{P}$ or As)



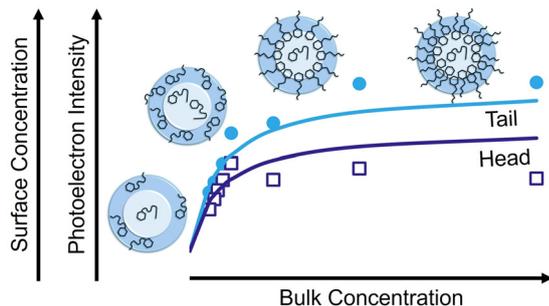
● Ba ● Ge ● Pn (P or As)



BaGe_2P_2 and BaGe_2As_2 pnictides as promising ferroelectric semiconductors for thin film solar cell

Purun-hanul Kim, Seungwu Han and Youngho Kang*

17521



X-ray photoelectron spectroscopy of surfactants on sub-micron aqueous aerosols

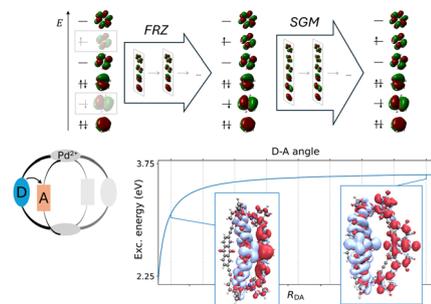
Alexandra M. Deal, Alexander M. Prophet, Sorren Warkander, Madison M. Foreman, Pyeongeun Kim, Daniel M. Neumark, Musahid Ahmed and Kevin R. Wilson*



17533

An improved guess for the variational calculation of charge-transfer excitations in large systems

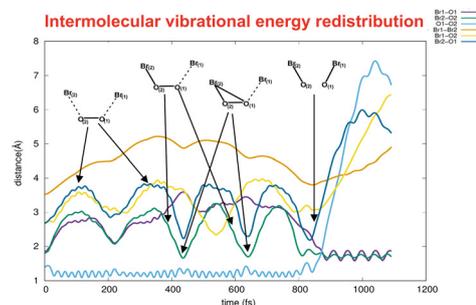
Nicola Bogo,* Zeyi Zhang, Martin Head-Gordon and Christopher J. Stein



17548

Photochemistry of dibromine peroxide, BrOOBr

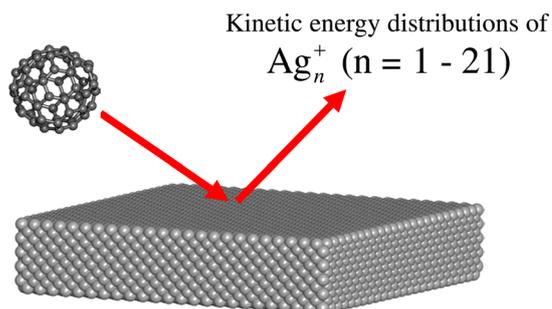
Wiem Chebbi,* Najoua Derbel, Thibaud Cours and Alexander Alijah



17557

Emission of velocity correlated clusters up to Ag_{21}^+ induced by keV C_{60}^- impacting a silver surface

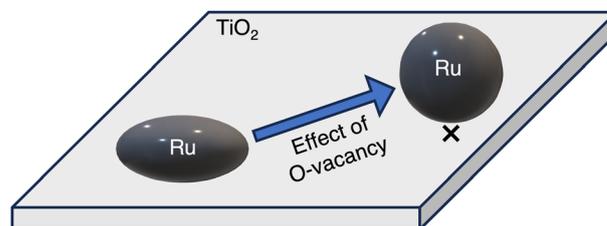
E. Armon, A. Bekkerman, B. Tsipinyuk and E. Kolodney*



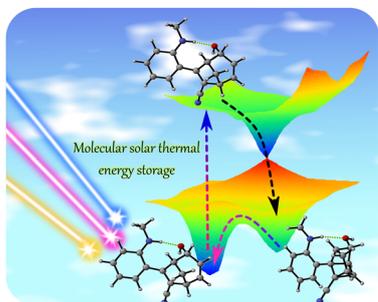
17564

Influence of oxygen vacancies on the morphology of Ru_{10} clusters supported on TiO_2

Joshua M. Sims and Carine Michel*



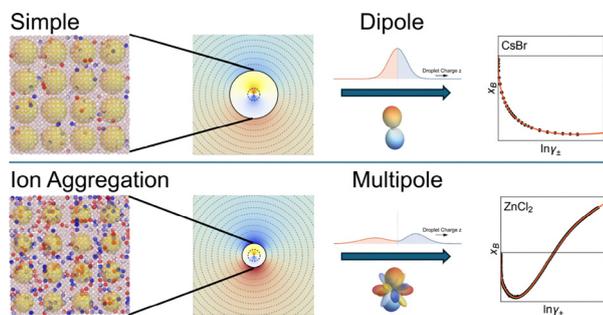
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H-bonding-assisted energy retention in bicyclic diene photoswitches for rechargeable solar thermal batteries: CASSCF, CASPT2, and DLPNO-CCSD(T) insights

Akanksha Ashok Sangolkar, Rama Krishna Kadiyam, Sibam Sahu and Ravinder Pawar*

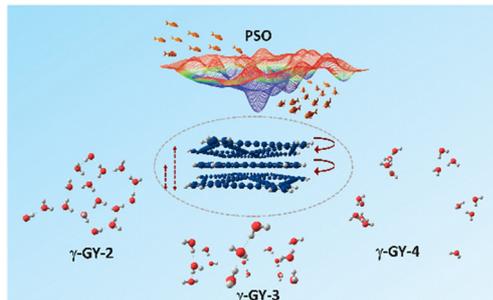
17585



A new perspective on aqueous electrolyte solutions

Gerhard Schwaab* and Simone Pezzotti*

17598



Leveraging metaheuristics to uncover water confinement in multilayer graphynes

Megha Rajeevan and Rotti Srinivasamurthy Swathi*

