

IN THIS ISSUE

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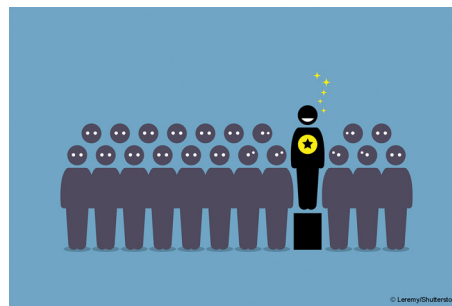
Cover

See Zhuwu Jiang,
Yuanmei Chen
et al., pp. 12129–12138.
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Phys. Chem. Chem. Phys.,
2025, 27, 12129.

EDITORIAL

12111

Outstanding Reviewers for *Physical Chemistry Chemical Physics* in 2024

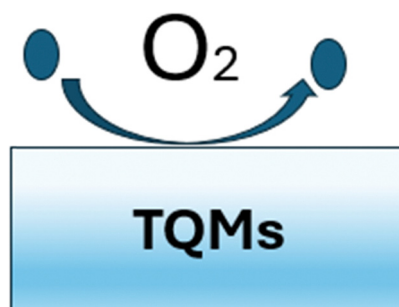


PERSPECTIVE

12112

Influence of surface oxidation on the catalytic activity of topological quantum materials

Ashraf Abdelrahman Assadig Elameen* and
Rowa Mahjoub Yahia Elhassan



Environmental Science: Atmospheres

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Fundamental questions
Elemental answers

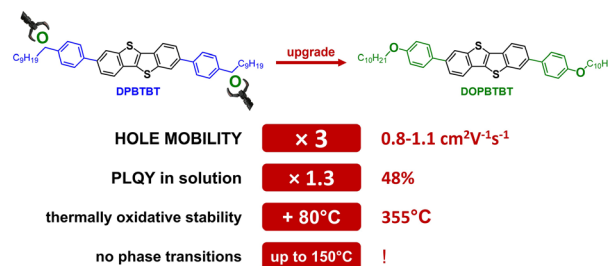


COMMUNICATION

12119

Decyloxy-substituted BTBT derivatives for highly efficient and stable thin-film organic (opto)electronic devices

Roman S. Fedorenko, Liya A. Poletavkina, Vasily A. Trukhanov, Konstantin N. Kuklin, Dmitry O. Balakirev, Ivan V. Dyadishchev, Nikita S. Saratovsky, Artem V. Bakirov, Sergei A. Ponomarenko, Yuriy N. Luponosov,* Dmitry Yu. Paraschuk* and Andrey Yu. Sosorev*

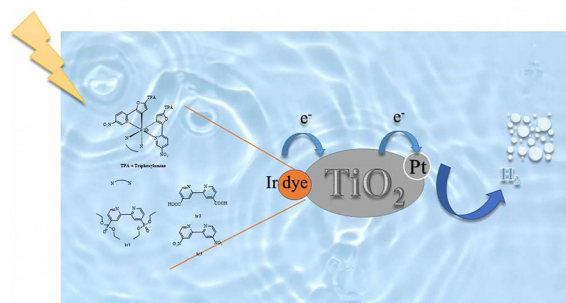


RESEARCH PAPERS

12129

Effect of anchoring groups on the photocatalytic performance of iridium(III) complexes in hydrogen production and their toxicological analysis

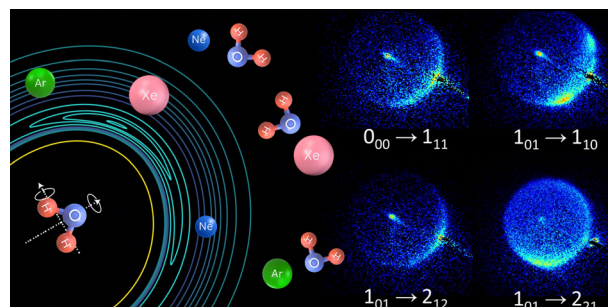
Xiao Yao, Linyu Fan, Zhuwu Jiang,* Chaoqun Zheng, Jinfeng Chen, Yachen Jiang, Yisang Lu, Cheuk-Lam Ho and Yuanmei Chen*



12139

A comprehensive study of the differential cross sections for water–rare gas collisions: experimental and theoretical perspectives

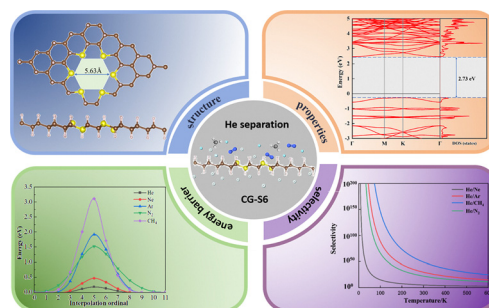
Ricardo Manuel García-Vázquez,* Zhong-Fa Sun,* Chung-Hsin Yang, Lisán David Cabrera-González, Otoniel Denis-Alpizar, Philippe Halvick, David H. Parker* and Thierry Stoecklin*



12152

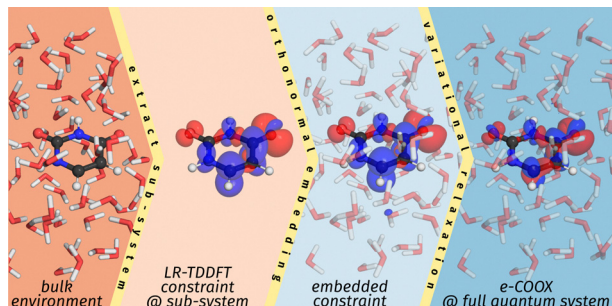
Sulfur-doped crown ether graphene for enhanced helium separation

Qinglan Zhao, Yingying Fu, Xiaxia Gong, Wenming Lu, Lin Dai, Wei Liu* and Jing Xu*



RESEARCH PAPERS

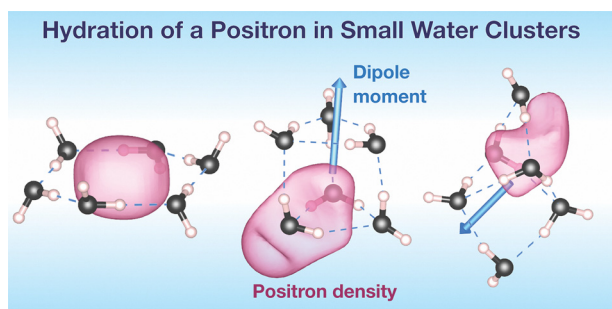
12161



An embedding scheme for constraint-based orbital-optimized excitations in molecular and bulk environments

Yannick Lemke, Jörg Kussmann* and Christian Ochsenfeld*

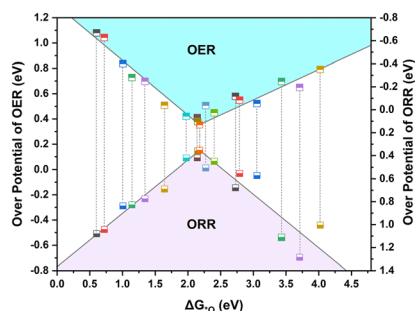
12171



Applications of the density functional method combined with the electron–positron correlation–polarization potential to positron binding to hydrocarbons and water clusters

Daisuke Yoshida,* Toshiyuki Takayanagi, Yukiumi Kita, Tomomi Shimazaki and Masanori Tachikawa

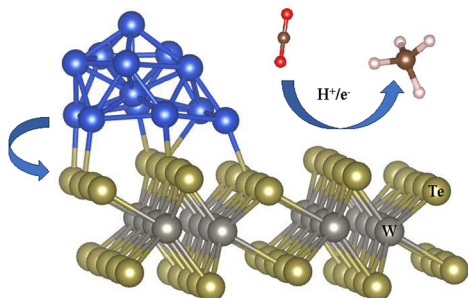
12182



Rational design of bifunctional OER/ORR metal-free catalysts based on boron-doped graphene by strain engineering

Jun Zhou, Yujia Cheng, Yuping Ren, Mo Xiong, Haozhen Dou, Yi Jiang, Luyuan Wang,* Chuangwei Liu* and Wenjun Tang*

12190



Enhancing electrocatalytic CO₂ reduction via engineering substrate–cluster interaction

Qian Sun, Huiru Yang,* Chunmei Zhang* and Aijun Du

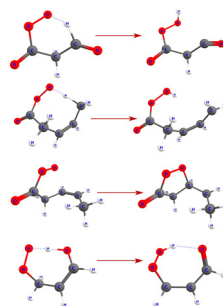


RESEARCH PAPERS

12198

Rapid unimolecular reactions of acyl peroxy radicals: extending the structure–activity relationships

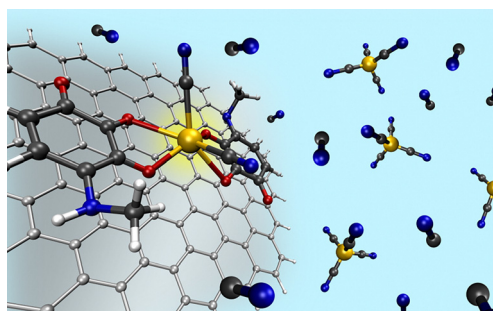
Lauri Franzon,* Anni Savolainen, Siddharth Iyer, Matti Rissanen and Theo Kurtén*



12211

Rational design of electrochemical sensors based on quinone derivatives adsorbed on graphene for the detection of $[\text{Cd}(\text{CN})_4]^{2-}$

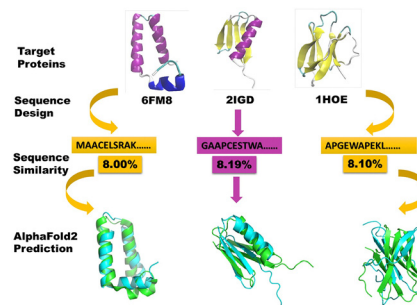
Golfer Muedas-Taípe,* Michael Badawi, Angélica María Baena-Moncada and Miguel Ponce-Vargas*



12220

Preserving structural integrity: fold reproducibility in computational design of proteins non-homologous to wild-type sequences

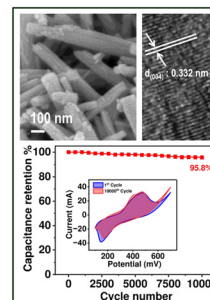
Bondeepa Saikia and Anupaul Baruah*



12231

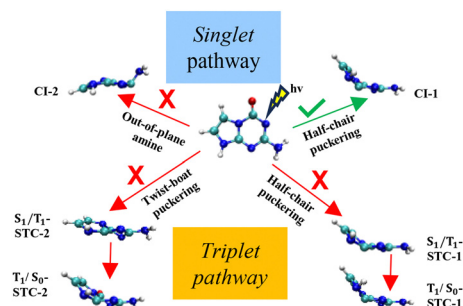
Hydrothermally synthesized 2H-WS₂ nanorods for improved supercapacitor electrode performance

Somveer, Rohit Yadav, Jitesh Pani, Rakesh Nanna, Ranjit Kumar, Vinay S. Palaparthi, Kusum Kumari, Davender Singh, Dharamvir Singh Ahlawat,* Hitesh Borkar* and Jitendra Gangwar*



RESEARCH PAPERS

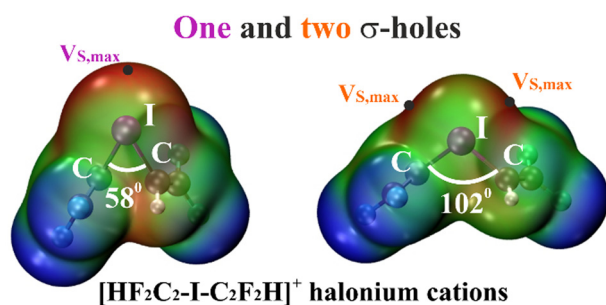
12240



Efficient photodeactivation mechanism in an unnatural nucleic acid base

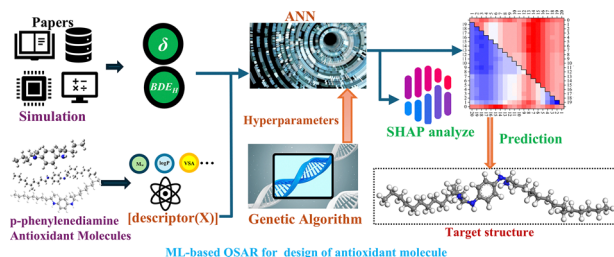
Somsuta Ray and Debashree Ghosh*

12248

Arrangement of σ -holes at the halogen atom in halonium cations

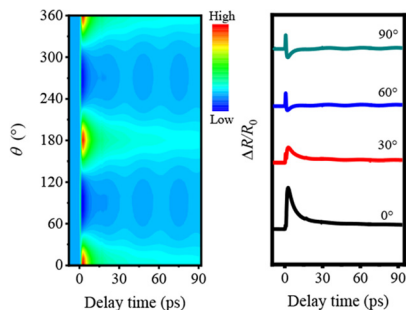
Mariusz Michalczyk* and Wiktor Zierkiewicz

12256

Machine learning-assisted design of the molecular structure of *p*-phenylenediamine antioxidants

Zongya Wu, Shuai Sun, Chaokun Huang, Li Zhou, Yanlong Luo and Xiujuan Wang*

12267



Anisotropic ultrafast hot carrier dynamics of two-dimensional SnS single crystals

Zanxiong Peng, Borong Cong, Jiajun Cao, Chunlian Li, Xiaodong Shen and Weizheng Liang*



Specific features of the spin density distribution and magnetic properties in a series of pyrazolyl-substituted nitronyl nitroxides: a magnetochemical and quantum chemical study

SPIN LABEL POSITION MATTERS

NN-4PzEt NN-5PzEt



IN THIS STUDY:

- spin density distribution
- supramolecular effects
- magnetic properties

Excitations in lanthanide ions: a systematic evaluation of two-component CAS-Cl and GW

Interplay between intrinsic defects and optoelectronic properties of semi-Heusler gapped metals

Figure 1 consists of two panels. The left panel is a ternary phase diagram for the Nb-Co-Sb system. The vertices are labeled Nb, Co, and Sb. The axes are marked from 0.0 to 1.0. A green dot is located at the top vertex (Sb) and a red dot is located at the bottom vertex (Co). A green line connects the two dots. A green arrow points from the red dot to the green line, labeled $Nb_{0.8}CoSb$. The right panel is a plot of the absorption coefficient (in units of 10^6 cm^{-1}) versus energy (in eV) for various compositions. The x-axis ranges from 0.0 to 3.0 eV, and the y-axis ranges from 0.0 to 1.0. The legend indicates the following compositions: $NbCoSb$ (black), $Nb_{0.95}CoSb$ (blue), $Nb_{0.9}CoSb$ (green), $Nb_{0.85}CoSb$ (red), and $Nb_{0.8}CoSb$ (magenta). The curves show a sharp increase in absorption coefficient starting around 1.5 eV, reaching a plateau around 2.5 eV.

Computational high-throughput screening of high-performance transition metal C₈N₈ single-atom electrocatalysts for the oxygen reduction reaction

The figure illustrates the design process of a sustainable material, starting from a molecular structure and a periodic table, leading to a funnel diagram of sustainability factors, and finally to a molecular structure with a central transition metal atom.

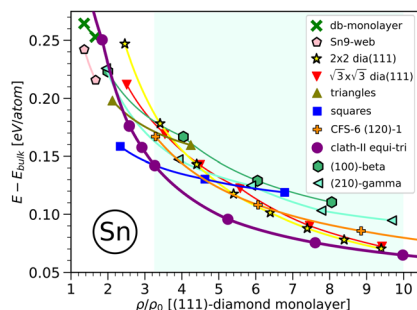
Top Left: A molecular structure diagram showing a central yellow sphere (Transition Metal, TM) surrounded by blue spheres (Carbon, C) and purple spheres (Oxygen, O).

Top Right: A periodic table highlighting elements categorized by risk factors:

- Radioactive and/or synthetic:** Elements 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, 160, 161, 162, 163, 164, 165, 166, 167, 168, 169, 170, 171, 172, 173, 174, 175, 176, 177, 178, 179, 180, 181, 182, 183, 184, 185, 186, 187, 188, 189, 190, 191, 192, 193, 194, 195, 196, 197, 198, 199, 200, 201, 202, 203, 204, 205, 206, 207, 208, 209, 210, 211, 212, 213, 214, 215, 216, 217, 218, 219, 220, 221, 222, 223, 224, 225, 226, 227, 228, 229, 230, 231, 232, 233, 234, 235, 236, 237, 238, 239, 240, 241, 242, 243, 244, 245, 246, 247, 248, 249, 250, 251, 252, 253, 254, 255, 256, 257, 258, 259, 260, 261, 262, 263, 264, 265, 266, 267, 268, 269, 270, 271, 272, 273, 274, 275, 276, 277, 278, 279, 280, 281, 282, 283, 284, 285, 286, 287, 288, 289, 290, 291, 292, 293, 294, 295, 296, 297, 298, 299, 300, 301, 302, 303, 304, 305, 306, 307, 308, 309, 310, 311, 312, 313, 314, 315, 316, 317, 318, 319, 320, 321, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 336, 337, 338, 339, 340, 341, 342, 343, 344, 345, 346, 347, 348, 349, 350, 351, 352, 353, 354, 355, 356, 357, 358, 359, 360, 361, 362, 363, 364, 365, 366, 367, 368, 369, 370, 371, 372, 373, 374, 375, 376, 377, 378, 379, 380, 381, 382, 383, 384, 385, 386, 387, 388, 389, 390, 391, 392, 393, 394, 395, 396, 397, 398, 399, 400, 401, 402, 403, 404, 405, 406, 407, 408, 409, 410, 411, 412, 413, 414, 415, 416, 417, 418, 419, 420, 421, 422, 423, 424, 425, 426, 427, 428, 429, 430, 431, 432, 433, 434, 435, 436, 437, 438, 439, 440, 441, 442, 443, 444, 445, 446, 447, 448, 449, 450, 451, 452, 453, 454, 455, 456, 457, 458, 459, 460, 461, 462, 463, 464, 465, 466, 467, 468, 469, 470, 471, 472, 473, 474, 475, 476, 477, 478, 479, 480, 481, 482, 483, 484, 485, 486, 487, 488, 489, 490, 491, 492, 493, 494, 495, 496, 497, 498, 499, 500, 501, 502, 503, 504, 505, 506, 507, 508, 509, 510, 511, 512, 513, 514, 515, 516, 517, 518, 519, 520, 521, 522, 523, 524, 525, 526, 527, 528, 529, 530, 531, 532, 533, 534, 535, 536, 537, 538, 539, 540, 541, 542, 543, 544, 545, 546, 547, 548, 549, 550, 551, 552, 553, 554, 555, 556, 557, 558, 559, 560, 561, 562, 563, 564, 565, 566, 567, 568, 569, 570, 571, 572, 573, 574, 575, 576, 577, 578, 579, 580, 581, 582, 583, 584, 585, 586, 587, 588, 589, 590, 591, 592, 593, 594, 595, 596, 597, 598, 599, 600, 601, 602, 603, 604, 605, 606, 607, 608, 609, 610, 611, 612, 613, 614, 615, 616, 617, 618, 619, 620, 621, 622, 623, 624, 625, 626, 627, 628, 629, 630, 631, 632, 633, 634, 635, 636, 637, 638, 639, 640, 641, 642, 643, 644, 645, 646, 647, 648, 649, 650, 651, 652, 653, 654, 655, 656, 657, 658, 659, 660, 661, 662, 663, 664, 665, 666, 667, 668, 669, 670, 671, 672, 673, 674, 675, 676, 677, 678, 679, 680, 681, 682, 683, 684, 685, 686, 687, 688, 689, 690, 691, 692, 693, 694, 695, 696, 697, 698, 699, 700, 701, 702, 703, 704, 705, 706, 707, 708, 709, 710, 711, 712, 713, 714, 715, 716, 717, 718, 719, 720, 721, 722, 723, 724, 725, 726, 727, 728, 729, 730, 731, 732, 733, 734, 735, 736, 737, 738, 739, 740, 741, 742, 743, 744, 745, 746, 747, 748, 749, 750, 751, 752, 753, 754, 755, 756, 757, 758, 759, 760, 761, 762, 763, 764, 765, 766, 767, 768, 769, 770, 771, 772, 773, 774, 775, 776, 777, 778, 779, 780, 781, 782, 783, 784, 785, 786, 787, 788, 789, 790, 791, 792, 793, 794, 795, 796, 797, 798, 799, 800, 801, 802, 803, 804, 805, 806, 807, 808, 809, 810, 811, 812, 813, 814, 815, 816, 817, 818, 819,

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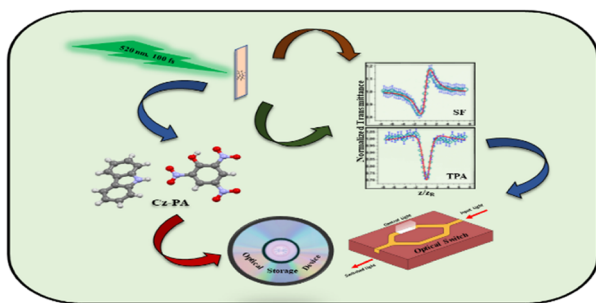
12313



Stable thin clathrate layers

Eva Pospíšilová

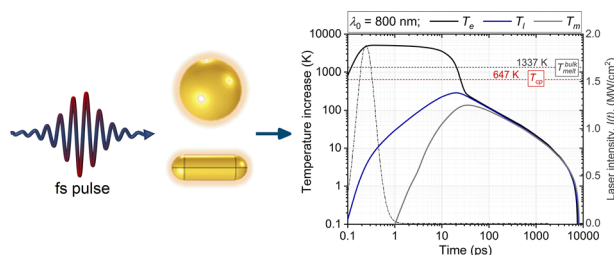
12331



Enhanced ultrafast cubic nonlinearity in the carbazole–picric acid complex for potential applications in photonic devices: Kerr nonlinearity with two-photon absorption

Mohd Mehkoom, Farman Ali, Amit Kumar Pradhan, Prasanta Kumar Datta* and Umakanta Tripathy*

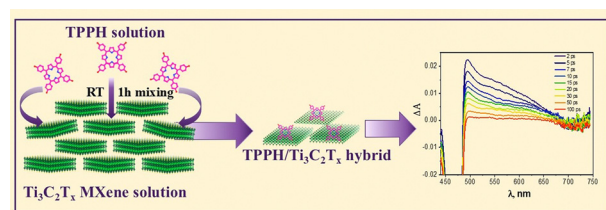
12343



Probing ultrafast heat transfer mechanisms in plasmonic gold nanostructures: FEM analysis of core–shell configurations under femtosecond laser irradiation

Joshua Fernandes and Myoung-Jin Kim*

12368



Coupling porphyrin with MXene nanosheets: exploring non-covalent interactions and photophysical characteristics

Marina Smirnova, Blazej Scheibe, Marcin Jarek, Alexandra Siklitskaya, Adam Kubas and Anna Lewandowska-Andralojc*

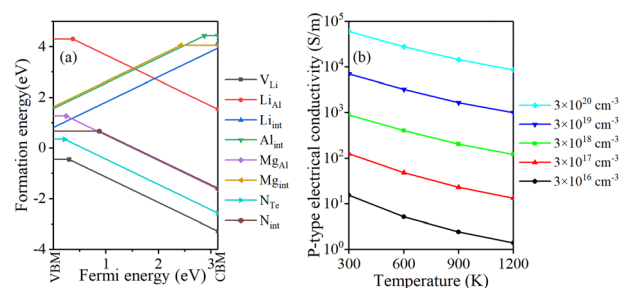


RESEARCH PAPERS

12381

A hybrid functional method for screening the p-type defects in wide gap semiconductor α -LiAlTe₂

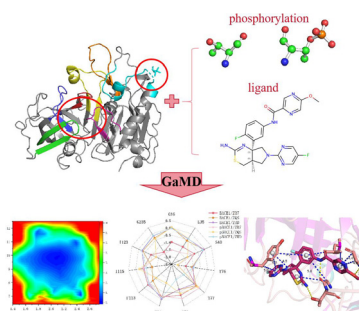
Shuaiwei Fan,* Jiayuan Wang, Yuhang Deng and Liu Yang



12389

Molecular mechanism of phosphorylation-mediated impacts on the conformation dynamics of ligand-bound BACE1 probed by Gaussian accelerated molecular dynamics

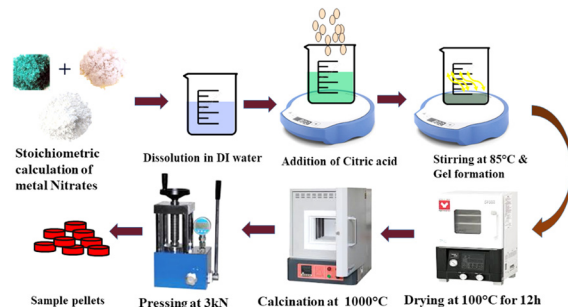
Chaoyue Jia, Yanqi Sun, Jianzhong Chen* and Xinguo Liu*



12405

A study on the role of moderate optical band gap energy in dielectric properties of NiFe₂O₄ nanoparticles by Ce ion doping for electronic device applications: the effect of doping concentration

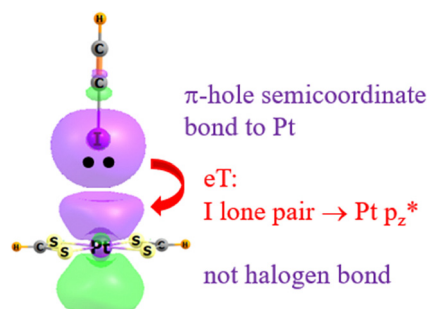
Abdulrahman I. Alharthi, Awais Khalid,* Pervaiz Ahmad, Arshad Ali, Shahroz Saleem* and Muhammad Adnan Munir*



12416

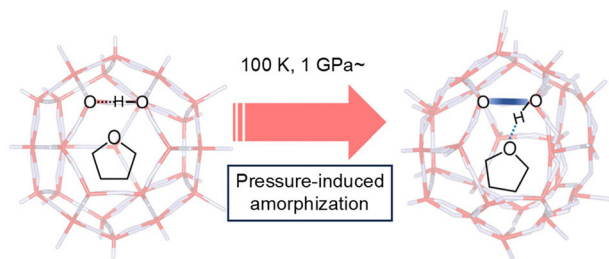
Semicoordinate and halogen bonding to group 10 and group 8 metals

Steve Scheiner



RESEARCH PAPERS

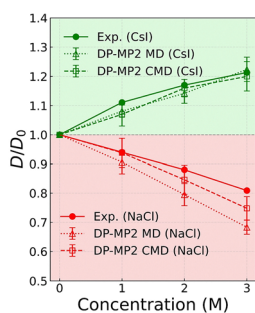
12427



Similarities between the tetrahydrofuran clathrate hydrate after pressure-induced amorphization and aqueous tetrahydrofuran solution: an *in situ* Raman and infrared spectroscopic study

Naoki Noguchi,* Haruki Fujii and Hidekazu Okamura

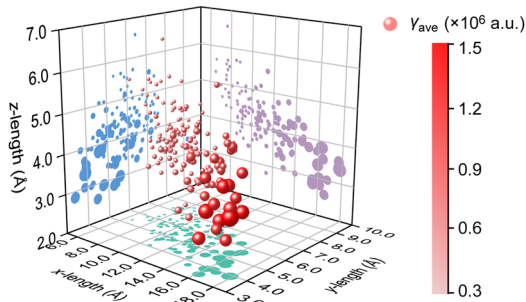
12438



Structure making and breaking effects of ions on the anomalous diffusion of water revealed by machine learning potentials

Jinfeng Liu,* Xuchao Zhou and Xiao He*

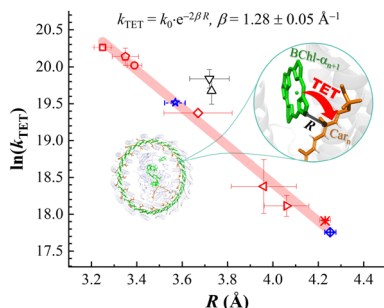
12453



A length descriptor to measure the linear and third-order nonlinear optical responses of atomic-cluster isomers

Quanjie Zhong

12462



Triplet excitation dynamics of photosynthetic light-harvesting antennae: mechanistic insights into the conjugation regulated carotenoid functionality

Yu-Qian Li, Yi-Hao Yan, Rong-Yao Gao, Jian-Wei Zou, Yu-Lu Wu, Xing-Yu Yue, Yao Lu, Xiang-Ping Wang, Ming-Qing Chen, Qi-Wei Li, Hao-Yi Wang, Peng Wang, Long-Jiang Yu,* Junrong Zheng and Jian-Ping Zhang*

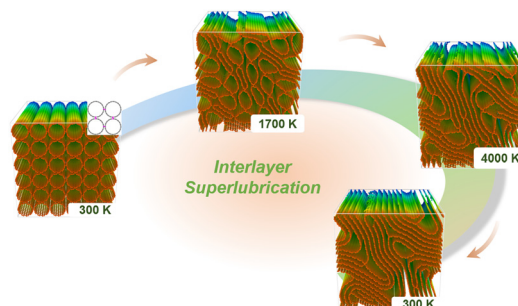


RESEARCH PAPERS

12474

Inter-layer superlubricity in a carbon nanotube array induced by high-temperature annealing

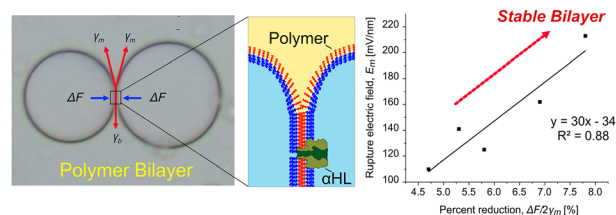
Yunlong Fan, Yushun Zhao,* Kaiyi Zheng, Yingxia He, Chao Sui, Xiaodong He and Chao Wang



12483

Reconstitution of nanopores in bilayers of diblock and triblock copolymers

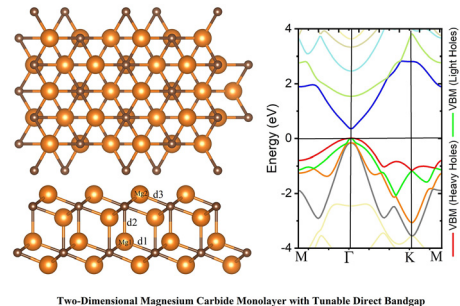
Hiroaki Kihara, Mikiyoshi Sato and Ryuji Kawano*



12494

First-principles investigation of a two-dimensional magnesium carbide monolayer: tunable bandgap, light carriers, and strain-induced topological and semiconductor-to-metal transitions

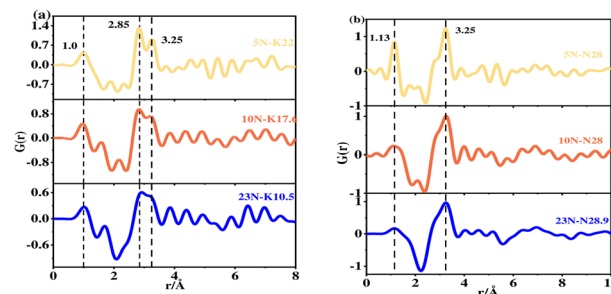
Mosayeb Naseri,* Shahram Yalameha and Sergey Gusarov



12507

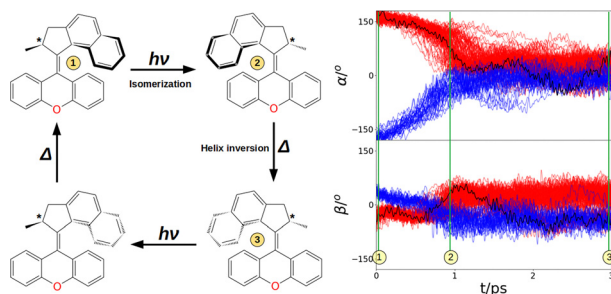
Study on the effect of NH₃ on the solubility of KCl and NH₄Cl: a microscopic view

Ao Wang, Xiaofu Guo, Fei Li,* Jie Liu, Mengdan Qiao, Zihan Xing, Yingying Zhao, Shizhao Wang, Panpan Zhang, Jingtao Bi, Jing Wang, Junsheng Yuan and Zhiyong Ji



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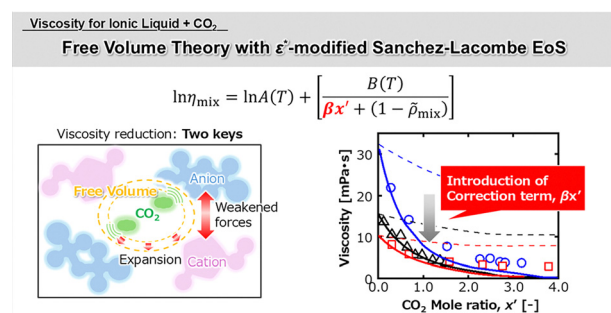
12519



First principles prediction of wavelength-dependent isomerization quantum yields of a second-generation molecular nanomotor

Jesús Lucia-Tamudo, Michelle Menkel-Lantz and Enrico Tapavicza*

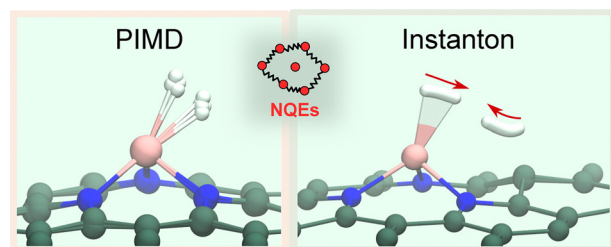
12532



Viscosity prediction of CO₂-saturated imidazolium-based ionic liquids using the ε*-modified Sanchez-Lacombe equation of state and free volume theory with a new correction term

Ryohei Otani, Yuya Hiraga* and Masaru Watanabe*

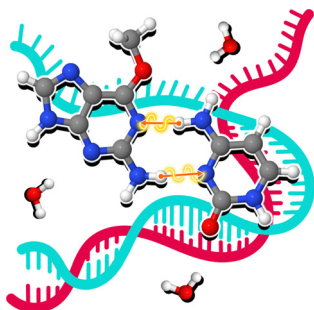
12542



Nuclear quantum effects in two-hydrogen intermediates on graphene-embedded transition metal atoms

Erxun Han, Wei Fang* and Ji Chen*

12550



Proton transfer in methylated G-C: nuclear quantum effects and water-assisted hopping

Juliana G. de Abrantes,* Adam P. Motala, Ian Riddlestone, Louie Slocombe and Marco Sacchi*

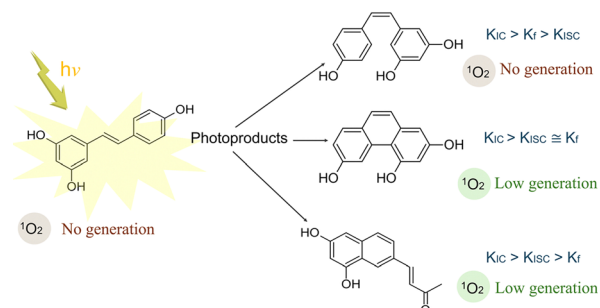


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Photophysics of resveratrol derivatives for singlet oxygen formation

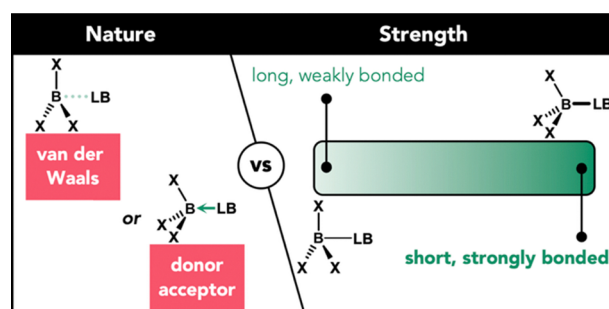
Mariana Yoshinaga, Josene M. Toldo, Willian R. Rocha* and Mario Barbatti*



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The spectrum from van der Waals to donor–acceptor bonding

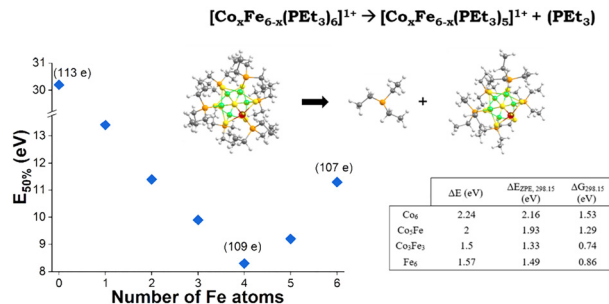
Daniela Rodrigues Silva,* Lucas de Azevedo Santos, Matthijs A. J. G. Koning, Céla Fonseca Guerra and Trevor A. Hamlin*



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Effect of heteroatom incorporation on electronic communication in metal chalcogenide nanoclusters

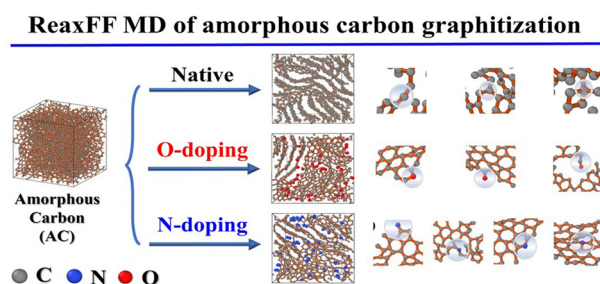
Shana Havenridge, Xilai Li, Julia Laskin* and Cong Liu*



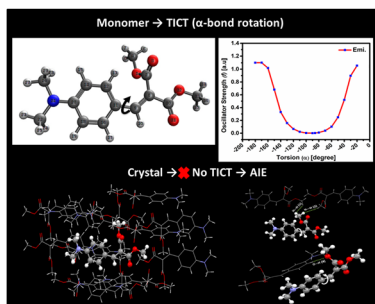
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ReaxFF MD simulations of graphitization of intact and O,N-doped amorphous carbon

Yiru Bian, Wentao Zhang, Tao Wu* and Dongqi Wang*



12593



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Aarzo, Kenichiro Saita, Masato Kobayashi, Takao Tsuneda,* Tetsuya Taketsugu and Ram Kinkar Roy*

