图书情报专题研究

最新学科研究热点与前沿

（2019）

第1期

西北工业大学图书馆

2019年4月

前　言

《图书情报专题研究》的宗旨是为我校师生开展学术研究提供有价值的参考信息，此项工作由图书馆信息咨询与发展研究部承担。“最新学科研究热点与前沿”根据学校所购买的数字资源，通过分析其深层次的功能，从数据库中组织整理出了与我校学科领域相关的最新学科热点研究论文、最新研究前沿及最新国际会议信息等，以期能对我校师生开展学术研究、项目立项、开题等学术研究活动提供帮助。

本期收集整理了如下七个方面的热点文献和前沿信息：

1、Nature Latest Research，Nature Chemistry 最新研究进展；

2、IEL Top25，IEL 数据库下载最多的 25 篇论文；

3、ESI（Essential Science Indicators）HOT PAPERS，按照 ESI 某一学科热点论文被引频次排名选取前 25 篇；

4、ESI（Essential Science Indicators）HIGHLY CITED PAPERS，按照 ESI 某一学科高被引论文被引频次排名选取前 25 篇；

5、AIAA、AAS、IAF 最新会议，由 AIAA、AAS、IAF 主站提供的最新会议信息，可供相关研究者参考；

6、ACM 最新会议，根据 ACM 主页所提供的最新会议信息整理所得，可供相关研究者参考；

7、IQPC 最新会议，由国际质量与竞争力中心（IQPC：International Quality and Productivity Center）提供的最新国际会议，内容涉及国防、能源、工业、科技、电信等领域。IQPC 是国际顶级的会议展览策划公司，于 1973 年成立于美国，旨在为全球业务主管提供量身定制的会议、大型会展以及培训课程，积极为行业人士的相互交流创建平台，使业内人士能够随时掌握行业发展的最新趋势及技术创新。

如果您对我们的栏目设置、内容编排、出版方式等有好的意见和建议，欢迎与我们联系，我们将积极采纳，使这份电子刊物日臻完善，共同为把我校建成学科特色鲜明的世界一流大学而努力。

图书馆

2019 年 4 月

目　录

NatureLatest Research(Chemistry)

来源：https://www.nature.com/nchem/

1. **标题：**Braiding, branching and chiral amplification of nanofibres in supramolecular gels
作者：Christopher D. Jones, Henry T. D. Simmons, Kate E. Horner, Kaiqiang Liu, Richard L. Thompson & Jonathan W. Steed
摘要：Helical nanofibres play key roles in many biological processes. Entanglements between helices can aid gelation by producing thick, interconnected fibres, but the details of this process are poorly understood. Here, we describe the assembly of an achiral oligo(urea) peptidomimetic compound into supramolecular helices. Aggregation of adjacent helices leads to the formation of fibrils, which further intertwine to produce high-fidelity braids with periodic crossing patterns. A braid theory analysis suggests that braiding is governed by rigid topological constraints, and that branching occurs due to crossing defects in the developing braids. Mixed-chirality helices assemble into relatively complex, odd-stranded braids, but can also form helical bundles by undergoing inversions of chirality. The oligo(urea) assemblies are also highly sensitive to chiral amplification, proposed to occur through a majority-rules mechanism, whereby trace chiral materials can promote the formation of gels containing only homochiral helices.
链接：https://www.nature.com/articles/s41557-019-0222-0

2. **标题：**α -Fluorination of carbonyls with nucleophilic fluorine
作者：Pauline Adler, Christopher J. Teskey, Daniel Kaiser, Marion Holy, Harald H. Sitte & Nuno Maulide
摘要：Given the unique properties of fluorine, and the ability of fluorination to change the properties of organic molecules, there is significant interest from medicinal chemists in innovative methodologies that enable the synthesis of new fluorinated motifs. State-of-the-art syntheses of α-fluorinated carbonyl compounds invariably rely on electrophilic fluorinating agents, which can be strongly oxidizing and difficult to handle. Here we show that reversing the polarity of the enolate partner to that of an enolonium enables nucleophilic fluorinating agents to be used for direct chemoselective α-C–H-fluorination of amides. Reduction of these products enables facile access to β-fluorinated amines and the value of this methodology is shown by the easy preparation of a number of fluorinated analogues of drugs and agrochemicals. A fluorinated analogue of citalopram, a marketed antidepressant drug, is presented as an example of the preserved biological activity after fluorination.
链接：https://www.nature.com/articles/s41557-019-0215-z

3.**标题：**Ion-mediated hydrogen-bond rearrangement through tunnelling in the iodide–dihydrate complex
作者：Pushp Bajaj, Jeremy O. Richardson & Francesco Paesani

摘要：A microscopic picture of hydrogen-bond structure and dynamics in ion hydration shells remains elusive. Small ion–dihydrate molecular complexes are ideal systems with which to investigate the interplay and competition between ion–water and water–water interactions. Here, state-of-the-art quantum dynamics simulations provide evidence for tunnelling in hydrogen-bond rearrangements in the iodide–dihydrate complex and show that it can be controlled through isotopic substitutions. We find that the iodide ion weakens the neighbouring water–water hydrogen bond, leading to faster water reorientation than in the analogous water trimer. These faster dynamics, which are apparently at odds with the slowdown observed in the first hydration shell of iodide in solution, can be traced back to the presence of a free OH bond in the iodide–dihydrate complex, which effectively triggers the overall structural rearrangements within it. Besides providing indirect support for cooperative hydrogen-bond dynamics in iodide solutions, the analysis presented here suggests that iodide ions may accelerate hydrogen-bond rearrangements at aqueous interfaces, where neighbouring water molecules can be undercoordinated.

链接：https://www.nature.com/articles/s41557-019-0220-2

4.**标题：**Non-chemisorbed gold–sulfur binding prevails in self-assembled monolayers

作者：Michael S. Inkpen, Zhen–Fei Liu, Haixing Li, Luis M. Campos, Jeffrey B. Neaton & Latha Venkataraman

摘要：Gold–thiol contacts are ubiquitous across the physical and biological sciences in connecting organic molecules to surfaces. When thiols bind to gold in self-assembled monolayers (SAMs) the fate of the hydrogen remains a subject of profound debate—with implications for our understanding of their physical properties, spectroscopic features and formation mechanism(s). Exploiting measurements of the transmission through a molecular junction, which is highly sensitive to the nature of the molecule–electrode contact, we demonstrate here that the nature of the gold–sulfur bond in SAMs can be probed via single-molecule conductance measurements. Critically, we find that SAM measurements of dithiol-terminated molecular junctions yield a significantly lower conductance than solution measurements of the same molecule. Through numerous control experiments, conductance noise analysis and transport calculations based on density functional theory, we show that the gold–sulfur bond in SAMs prepared from the solution deposition of dithiols does not have chemisorbed character, which strongly suggests that under these widely used preparation conditions the hydrogen is retained.

链接：https://www.nature.com/articles/s41557-019-0216-y

5.**标题：**Fluorogenic D-amino acids enable real-time monitoring of peptidoglycan biosynthesis and high-throughput transpeptidation assays

作者：Yen-Pang Hsu, Edward Hall, Garrett Booher, Brennan Murphy, Atanas D. Radkov, Jacob Yablonowski, Caitlyn Mulcahey, Laura Alvarez, Felipe Cava, Yves V. Brun, Erkin Kuru & Michael S. VanNieuwenhze

摘要：Peptidoglycan is an essential cell wall component that maintains the morphology and viability of nearly all bacteria. Its biosynthesis requires periplasmic transpeptidation reactions, which construct peptide crosslinkages between polysaccharide chains to endow mechanical strength. However, tracking the transpeptidation reaction in vivo and in vitro is challenging, mainly due to the lack of efficient, biocompatible probes. Here, we report the design, synthesis and application of rotor-fluorogenic D-amino acids (RfDAAs), enabling real-time, continuous tracking of transpeptidation reactions. These probes allow peptidoglycan biosynthesis to be monitored in real time by visualizing transpeptidase reactions in live cells, as well as real-time activity assays of D,D- and L,D-transpeptidases and sortases in vitro. The unique ability of RfDAAs to become fluorescent when incorporated into peptidoglycan provides a powerful new tool to study peptidoglycan biosynthesis with high temporal resolution and prospectively enable high-throughput screening for inhibitors of peptidoglycan biosynthesis.

链接：https://www.nature.com/articles/s41557-019-0217-x

6.标题：An automated platform for the enzyme-mediated assembly of complex oligosaccharides

作者：Tiehai Li, Lin Liu, Na Wei, Jeong-Yeh Yang, Digantkumar G. Chapla, Kelley W. Moremen & Geert-Jan Boons

摘要：An automated platform that can synthesize a wide range of complex carbohydrates will greatly increase their accessibility and should facilitate progress in glycoscience. Here we report a fully automated process for enzyme-mediated oligosaccharide synthesis that can give easy access to different classes of complex glycans including poly-N-acetyllactosamine derivatives, human milk oligosaccharides, gangliosides and N-glycans. Our automated platform uses a catch and release approach in which glycosyltransferase-catalysed reactions are performed in solution and product purification is accomplished by solid phase extraction. We developed a sulfonate tag that can easily be installed and enables highly efficient solid phase extraction and product release using a single set of washing conditions, regardless of the complexity of the glycan. Using this custom-built synthesizer, as many as 15 reaction cycles can be performed in an automated fashion without a need for lyophilization or buffer exchange steps.

链接：https://www.nature.com/articles/s41557-019-0219-8

7.标题：Liquid–liquid phase separation during amphiphilic self-assembly

作者：Alessandro Ianiro, Hanglong Wu, Mark M. J. van Rijt, M. Paula Vena, Arthur D. A. Keizer, A. Catarina C. Esteves, Remco Tuinier, Heiner Friedrich, Nico A. J. M. Sommerdijk & Joseph P. Patterson

摘要：The self-assembly of amphiphilic molecules in solution is a ubiquitous process in both natural and synthetic systems. The ability to effectively control the structure and properties of these systems is essential for tuning the quality of their functionality, yet the underlying mechanisms governing the transition from molecules to assemblies have not been fully resolved. Here we describe how amphiphilic self-assembly can be preceded by liquid–liquid phase separation. The assembly of a model block co-polymer system into vesicular structures was probed through a combination of liquid-phase electron microscopy, self-consistent field computations and Gibbs free energy calculations. This analysis shows the formation of polymer-rich liquid droplets that act as a precursor in the bottom-up formation of spherical micelles, which then evolve into vesicles. The liquid–liquid phase separation plays a role in determining the resulting vesicles’ structural properties, such as their size and membrane thickness, and the onset of kinetic traps during self-assembly.

链接：https://www.nature.com/articles/s41557-019-0210-4

8.标题：An efficient, step-economical strategy for the design of functional metalloproteins

作者：Jonathan Rittle, Mackenzie J. Field, Michael T. Green & F. Akif Tezcan

摘要：The bottom-up design and construction of functional metalloproteins remains a formidable task

in biomolecular design. Although numerous strategies have been used to create new metalloproteins, pre-existing knowledge of the tertiary and quaternary protein structure is often required to generate suitable platforms for robust metal coordination and activity. Here we report an alternative and easily implemented approach (metal active sites by covalent tethering or MASCoT) in which folded protein building blocks are linked by a single disulfide bond to create diverse metal coordination environments within evolutionarily naive protein–protein interfaces. Metalloproteins generated using this strategy uniformly bind a wide array of first-row transition metal ions (MnII, FeII, CoII, NiII, CuII, ZnII and vanadyl) with physiologically relevant thermodynamic affinities (dissociation constants ranging from 700 nM for MnII to 50 fM for CuII). MASCoT readily affords coordinatively unsaturated metal centres—including a penta-His-coordinated non-haem Fe site—and well-defined binding pockets that can accommodate modifications and enable coordination of exogenous ligands such as nitric oxide to the interfacial metal centre.
链接：https://www.nature.com/articles/s41557-019-0218-9

9.**标题：**Maleimide–thiol adducts stabilized through stretching
作者：Wenmao Huang, Xin Wu, Xiang Gao, Yifei Yu, Hai Lei, Zhenshu Zhu, Yi Shi, Yulan Chen, Meng Qin, Wei Wang & Yi Cao
摘要：Maleimide–thiol reactions are widely used to produce protein–polymer conjugates for therapeutics. However, maleimide–thiol adducts are unstable in vivo or in the presence of thiol-containing compounds because of the elimination of the thiosuccinimide linkage through a retro-Michael reaction or thiol exchange. Here, using single-molecule force spectroscopy, we show that applying an appropriate stretching force to the thiosuccinimide linkage can considerably stabilize the maleimide–thiol adducts, in effect using conventional mechanochemistry of force-accelerated bond dissociation to unconventionally stabilize an adjacent bond. Single-molecule kinetic analysis and bulk structural characterizations suggest that hydrolysis of the succinimide ring is dominant over the retro-Michael reaction through a force-dependent kinetic control mechanism, and this leads to a product that is resistant to elimination. This unconventional mechanochemical approach enabled us to produce stable polymer–protein conjugates by simply applying a mechanical force to the maleimide–thiol adducts through mild ultrasonication. Our results demonstrate the great potential of mechanical force for stimulating important productive chemical transformations.
链接：https://www.nature.com/articles/s41557-018-0209-2

10.**标题：**Transition-metal-bridged bimetallic clusters with multiple uranium–metal bonds
作者：Genfeng Feng, Mingxing Zhang, Dong Shao, Xinyi Wang, Shuao Wang, Laurent Maron & Congqing Zhu
摘要：Heterometallic clusters are important in catalysis and small-molecule activation because of the multimetallic synergistic effects from different metals. However, multimetallic species that contain uranium–metal bonds remain very scarce due to the difficulties in their synthesis. Here we present a straightforward strategy to construct a series of heterometallic clusters with multiple uranium–metal bonds. These complexes were created by facile reactions of a uranium precursor with Ni(COD)2 (COD, cyclooctadiene). The multimetallic clusters' cores are supported by a heptadentate N4P3 scaffold. Theoretical investigations indicate the formation of uranium–nickel bonds in a U2Ni2 and a U2Ni3 species, but also show that they exhibit a uranium–uranium interaction; thus, the electronic configuration of uranium in these species is U(III)-5f26d1. This study provides further understanding

of the bonding between f-block elements and transition metals, which may allow the construction of d–f heterometallic clusters and the investigation of their potential applications.
链接：https://www.nature.com/articles/s41557-018-0195-4

11.**标题：**Mesopolymer synthesis by ligand-modulated direct arylation polycondensation towards n-type and ambipolar conjugated systems
作者：Zhenjie Ni, Hanlin Wang, Huanli Dong, Yanfeng Dang, Qiang Zhao, Xiaotao Zhang & Wenping Hu
摘要：Conjugated polymers are attractive components for plastic electronics, but their structural defects, low solubility and batch-to-batch variation—mainly in terms of molecular weight and dispersity—hinder practical applications. Here, we demonstrate that these issues can be circumvented by using conjugated mesopolymers, which have the advantages of both oligomers and polymers. A diketopyrrolopyrrole monomer and a benzothiadiazole derivative react through direct arylation polycondensation, promoted by sterically hindered adamantyl ligand coordinated palladium catalysts, to form mesopolymers. The reaction is facile, environmentally benign (it does not require tin or boron reagents) and occurs in high yields. The resulting mesopolymers have a strictly alternating donor–acceptor structure, without detectable homocoupling and β-arylation defects, and exhibit number-averaged molecular weights (Mn) between 1 and 10 kDa. They also show good solution processability and have significantly enhanced electron mobilities, which makes them n-type and ambipolar semiconductors, with advantages over their polymer counterparts.
链接：https://www.nature.com/articles/s41557-018-0200-y

12.**标题：**Copper atom-pair catalyst anchored on alloy nanowires for selective and efficient electrochemical reduction of CO2
作者：Jiqing Jiao, Rui Lin, Shoujie Liu, Weng-Chon Cheong, Chao Zhang, Zheng Chen, Yuan Pan, Jianguo Tang, Konglin Wu, Sung-Fu Hung, Hao Ming Chen, Lirong Zheng, Qi Lu, Xuan Yang, Bingjun Xu, Hai Xiao, Jun Li, Dingsheng Wang, Qing Peng, Chen Chen & Yadong Li
摘要：The electrochemical reduction of CO2 could play an important role in addressing climate-change issues and global energy demands as part of a carbon-neutral energy cycle. Single-atom catalysts can display outstanding electrocatalytic performance; however, given their single-site nature they are usually only amenable to reactions that involve single molecules. For processes that involve multiple molecules, improved catalytic properties could be achieved through the development of atomically dispersed catalysts with higher complexities. Here we report a catalyst that features two adjacent copper atoms, which we call an ‘atom-pair catalyst’, that work together to carry out the critical bimolecular step in CO2 reduction. The atom-pair catalyst features stable Cu10–Cu1x+ pair structures, with Cu1x+ adsorbing H2O and the neighbouring Cu10 adsorbing CO2, which thereby promotes CO2 activation. This results in a Faradaic efficiency for CO generation above 92%, with the competing hydrogen evolution reaction almost completely suppressed. Experimental characterization and density functional theory revealed that the adsorption configuration reduces the activation energy, which generates high selectivity, activity and stability under relatively low potentials.
链接：https://www.nature.com/articles/s41557-018-0201-x

13.**标题：**The formation of all-cis-(multi)fluorinated piperidines by a dearomatization–hydrogenation process

作者：Zackaria Nairoukh, Marco Wollenburg, Christoph Schlepphorst, Klaus Bergander & Frank Glorius

摘要：Piperidines and fluorine substituents are both independently indispensable components in pharmaceuticals, agrochemicals and materials. Logically, the incorporation of fluorine atoms into piperidine scaffolds is therefore an area of tremendous potential. However, synthetic approaches towards the formation of these architectures are often impractical. The diastereoselective synthesis of substituted monofluorinated piperidines often requires substrates with pre-defined stereochemistry. That of multifluorinated piperidines is even more challenging, and often needs to be carried out in multistep syntheses. In this report, we describe a straightforward process for the one-pot rhodium-catalysed dearomatization–hydrogenation of fluoropyridine precursors. This strategy enables the formation of a plethora of substituted all-cis-(multi)fluorinated piperidines in a highly diastereoselective fashion through pyridine dearomatization followed by complete saturation of the resulting intermediates by hydrogenation. Fluorinated piperidines with defined axial/equatorial orientation of fluorine substituents were successfully applied in the preparation of commercial drugs analogues. Additionally, fluorinated PipPhos as well as fluorinated ionic liquids were obtained by this dearomatization–hydrogenation process.

链接：https://www.nature.com/articles/s41557-018-0197-2

14.**标题:** Fast galvanic lithium corrosion involving a Kirkendall-type mechanism

作者：Dingchang Lin, Yayuan Liu, Yanbin Li, Yuzhang Li, Allen Pei, Jin Xie, William Huang & Yi Cui

摘要：Developing a viable metallic lithium anode is a prerequisite for next-generation batteries. However, the low redox potential of lithium metal renders it prone to corrosion, which must be thoroughly understood for it to be used in practical energy-storage devices. Here we report a previously overlooked mechanism by which lithium deposits can corrode on a copper surface. Voids are observed in the corroded deposits and a Kirkendall-type mechanism is validated through electrochemical analysis. Although it is a long-held view that lithium corrosion in electrolytes involves direct charge-transfer through the lithium–electrolyte interphase, the corrosion observed here is found to be governed by a galvanic process between lithium and the copper substrate—a pathway largely neglected by previous battery corrosion studies. The observations are further rationalized by detailed analyses of the solid–electrolyte interphase formed on copper and lithium, where the disparities in electrolyte reduction kinetics on the two surfaces can account for the fast galvanic process.

链接：https://www.nature.com/articles/s41557-018-0203-8

15.**标题：** A nucleophilic gold complex

作者：Jamie Hicks, Akseli Mansikkamäki, Petra Vasko, Jose M. Goicoechea & Simon Aldridge

摘要：Solid-state auride salts featuring the negatively charged Au– ion are known to be stable in the presence of alkali metal counterions. While such electron-rich species might be expected to be nucleophilic (in the same manner as I–, for example), their instability in solution means that this has not been verified experimentally. Here we report a two-coordinate gold complex (NON)AlAuPtBu3 (where NON is the chelating tridentate ligand

4,5-bis(2,6-diisopropylanilido)-2,7-di-tert-butyl-9,9-dimethylxanthene) that features a strongly polarized bond, Auδ—Alδ+. This is synthesized by reaction of the potassium aluminyl compound [K{Al(NON)}]2 with tBu3PAuI. Computational studies of the complex, including quantum theory of atoms in molecules charge analysis, imply a charge at gold (−0.82) that is in line with the relative electronegativities of the two metals (Au: 2.54; Al: 1.61 on the Pauling scale). Consistently, the complex is found to act as a nucleophilic source of gold, reacting with diisopropylcarbodiimide and CO2 to give the Au–C bonded insertion products (NON)Al(X2C)AuPtBu3 (X = NiPr, 4; X = O, 5).

链接：https://www.nature.com/articles/s41557-018-0198-1

16.**标题：**Catalytic transport of molecular cargo using diffusive binding along a polymer track

作者：Lifei Zheng, Hui Zhao, Yanxiao Han, Haibin Qian, Lela Vukovic, Jasmin Mecinović, Petr Král & Wilhelm T. S. Huck

摘要：Transport at the molecular scale is a prerequisite for the development of future molecular factories. Here, we have designed oligoanionic molecular sliders on polycationic tracks that exploit Brownian motion and diffusive binding to transport cargo without using a chemical fuel. The presence of the polymer tracks increases the rate of bimolecular reactions between modified sliders by over two orders of magnitude. Molecular dynamics simulations showed that the sliders not only diffuse, but also jump and hop surprisingly efficiently along polymer tracks. Inspired by acetyl-coenzyme A transporting and delivering acetyl groups in many essential biochemical processes, we developed a new and unconventional type of catalytic transport involving sliders (including coenzyme A) picking up, transporting and selectively delivering molecular cargo. Furthermore, we show that the concept of diffusive binding can also be utilized for the spatially controlled transport of chemical groups across gels. This work represents a new concept for designing functional nanosystems based on random Brownian motion.

链接：https://www.nature.com/articles/s41557-018-0204-7

17.**标题：**Supercharging enables organized assembly of synthetic biomolecules

作者：Anna J. Simon, Yi Zhou, Vyas Ramasubramani, Jens Glaser, Arti Pothukuchy, Jimmy Gollihar, Jillian C. Gerberich, Janelle C. Leggere, Barrett R. Morrow, Cheulhee Jung, Sharon C. Glotzer, David W. Taylor & Andrew D. Ellington

摘要：Symmetrical protein oligomers are ubiquitous in biological systems and perform key structural and regulatory functions. However, there are few methods for constructing such oligomers. Here we have engineered completely synthetic, symmetrical oligomers by combining pairs of oppositely supercharged variants of a normally monomeric model protein through a strategy we term ‘supercharged protein assembly’ (SuPrA). We show that supercharged variants of green fluorescent protein can assemble into a variety of architectures including a well-defined symmetrical 16-mer structure that we solved using cryo-electron microscopy at 3.47 Å resolution. The 16-mer is composed of two stacked rings of octamers, in which the octamers contain supercharged proteins of alternating charges, and interactions within and between the rings are mediated by a variety of specific electrostatic contacts. The ready assembly of this structure suggests that combining oppositely supercharged pairs of protein variants may provide broad opportunities for generating novel architectures via otherwise unprogrammed interactions.

链接：https://www.nature.com/articles/s41557-018-0196-3

18.标题：Author Correction: Sequence-defined multifunctional polyethers via liquid-phase synthesis with molecular sieving

作者：Ruijiao Dong, Ruiyi Liu, Piers R. J. Gaffney, Marc Schaepertoens, Patrizia Marchetti, Christopher M. Williams, Rongjun Chen & Andrew G. Livingston

摘要：In the version of this Article originally published, the authors inadvertently cited ref. 10 in two places in the first paragraph. They would like to clarify that it should not have been cited in the sentence that starts “Polymer chemists have employed strategies such as single monomer insertion...” as it mistakenly implied that the IEG+ method described in ref. 10 could not produce unimolecular polymers; it can do so, as was demonstrated in ref. 10. The authors would also like to clarify that ref. 10 should not have been cited in the sentence that starts “Moreover, solid-phase synthesis is generally difficult to scale up...", as it implied that ref. 10 uses solid-phase synthesis; it does not, and is a purely liquid-phase process. The citation of ref. 10 has now been removed from these two sentences, but has been included elsewhere in the first two paragraphs of the Article as follows. In the first paragraph, at the end of the sentence “In iterative synthesis, specific monomers are added one at a time, or as multiples, to the end of a growing polymer chain, then reaction debris is separated from the chain extended polymer, and the cycle is repeated using the next monomer in the sequence10–12.”; this sentence has been further amended to indicate multiple monomers can also be added. The reference has also been added to the end of the first sentence of the second paragraph, which starts “Consequently, liquid-phase iterative synthetic methods...”, and in the third sentence of that paragraph, which now starts “For example, Johnson10, Whiting....”.

链接：https://www.nature.com/articles/s41557-019-0212-2

19.标题：The reductive C3 functionalization of pyridinium and quinolinium salts through iridium-catalysed interrupted transfer hydrogenation

作者：Alexandru Grozavu, Hamish B. Hepburn, Philip J. Smith, Harish K. Potukuchi, Peter J. Lindsay-Scott & Timothy J. Donohoe

摘要：Aromatic rings are ubiquitous in organic chemistry and form the basis of many commercial products. Despite the numerous routes available for the preparation of aromatic compounds, there remain few methods that allow their conversion into synthetically useful partially saturated derivatives and even fewer that allow new C–C bonds to be formed at the same time. Here we set out to address this problem and uncover a unique catalytic partial reduction reaction that forms partially saturated azaheterocycles from aromatic precursors. In this reaction, methanol and formaldehyde are used for the reductive functionalization of pyridines and quinolines using catalytic iridium; thus, inexpensive and renewable feedstocks are utilized in the formation of complex N-heterocycles. By harnessing the formation of a nucleophilic enamine intermediate, the C–C bond-forming process reverses the normal pattern of reactivity and allows access to the C3 position of the arene. Mechanistic investigations using D-labelling experiments reveal the source of hydride added to the ring and show the reversible nature of the iridium-hydride addition.

链接：https://www.nature.com/articles/s41557-018-0178-5

20.标题：Chemoselective methylene oxidation in aromatic molecules

作者：Jinpeng Zhao, Takeshi Nanjo, Emilio C. de Lucca Jr & M. Christina White

摘要：Despite significant progress in the development of site-selective aliphatic C–H oxidations over the past decade, the ability to oxidize strong methylene C–H bonds in the presence of more oxidatively labile aromatic functionalities remains a major unsolved problem. Such chemoselective reactivity is highly desirable for enabling late-stage oxidative derivatizations of pharmaceuticals and medicinally important natural products that often contain such functionality. Here, we report a simple manganese small-molecule catalyst Mn(CF3–PDP) system that achieves such chemoselectivity via an unexpected synergy of catalyst design and acid additive. Preparative remote methylene oxidation is obtained in 50 aromatic compounds housing medicinally relevant halogen, oxygen, heterocyclic and biaryl moieties. Late-stage methylene oxidation is demonstrated on four drug scaffolds, including the ethinylestradiol scaffold where other non-directed C–H oxidants that tolerate aromatic groups effect oxidation at only activated tertiary benzylic sites. Rapid generation of a known metabolite (piragliatin) from an advanced intermediate is demonstrated.

链接：https://www.nature.com/articles/s41557-018-0175-8

21. **标题：**Carbopalladation of C–C σ-bonds enabled by strained boronate complexes

作者：Alexander Fawcett, Tobias Biberger & Varinder K. Aggarwal

摘要：Transition-metal-catalysed cross-coupling reactions, particularly those mediated by palladium, are some of the most broadly used chemical transformations. The fundamental reaction steps of such cross-couplings typically include oxidative addition, transmetallation, carbopalladation of a π-bond and/or reductive elimination. Herein, we describe an unprecedented fundamental reaction step: a C–C σ-bond carbopalladation. Specifically, an aryl palladium(II) complex interacts with a σ-bond of a strained bicyclo[1.1.0]butyl boronate complex to enable addition of the aryl palladium(II) species and an organoboronic ester substituent across a C–C σ-bond. The overall process couples readily available aryl triflates and organoboronic esters across a cyclobutane unit with total diastereocontrol. The pharmaceutically relevant 1,1,3-trisubstituted cyclobutane products are decorated with an array of modular building blocks, including a boronic ester that can be readily derivatized.

链接：https://www.nature.com/articles/s41557-018-0181-x

22. **标题：**Streamlining the chemoenzymatic synthesis of complex N-glycans by a stop and go strategy

作者：Lin Liu, Anthony R. Prudden, Chantelle J. Capicciotti, Gerlof P. Bosman, Jeong-Yeh Yang, Digantkumar G. Chapla, Kelley W. Moremen & Geert-Jan Boons

摘要：Contemporary chemoenzymatic approaches can provide highly complex multi-antennary N-linked glycans. These procedures are, however, very demanding and typically involve as many as 100 chemical steps to prepare advanced intermediates that can be diversified by glycosyltransferases in a branch-selective manner to give asymmetrical structures commonly found in nature. Only highly specialized laboratories can perform such syntheses, which greatly hampers progress in glycoscience. Here we describe a biomimetic approach in which a readily available bi-antennary glycopeptide can be converted in ten or fewer chemical and enzymatic steps into multi-antennary N-glycans that at each arm can be uniquely extended by glycosyltransferases to give access to highly complex asymmetrically branched N-glycans. A key feature of our approach is the installation of additional branching points using recombinant MGAT4 and MGAT5 in combination with unnatural sugar donors. At an appropriate point in the enzymatic synthesis, the unnatural monosaccharides can be converted into their natural counterpart, allowing each arm to be elaborated into a unique appendage.

链接：https://www.nature.com/articles/s41557-018-0188-3

23. **标题：**Intersystem crossing in the exit channel

作者：Hongwei Li, Alexander Kamasah, Spiridoula Matsika & Arthur G. Suits

摘要：Intersystem crossing plays an important role in photochemistry. It is understood to be efficient when heavy atoms are present due to strong spin–orbit coupling, or when strongly bound long-lived complexes are formed that increase the chance of finding the singlet–triplet intersection seam. Here we present evidence for a different intersystem crossing mechanism in the bimolecular reaction of O(3P) with alkylamines. In crossed-beam experiments, product velocity–flux maps are measured for aminoalkyl radicals produced from H abstraction from the methyl group, which also gives OH radicals as co-fragments. The low translational-energy release and isotropic angular distributions of the products indicate that such reactions undergo the formation of a complex before OH and aminoalkyl are produced. However, there is no well on the triplet potential energy surface that could support such a complex. Multi-reference ab initio calculations suggest, instead, that intersystem crossing occurs in the exit-channel region due to the long-range dipole–dipole interaction between the nascent radical product pair coupled with the vanishing singlet–triplet splitting at long range. Intersystem crossing then leads to a deep hydroxylamine well before OH elimination.

链接：https://www.nature.com/articles/s41557-018-0186-5

24. **标题：**Rapamycin-inspired macrocycles with new target specificity

作者：Zufeng Guo, Sam Y. Hong, Jingxin Wang, Shahid Rehan, Wukun Liu, Hanjing Peng, Manisha Das, Wei Li, Shridhar Bhat, Brandon Peiffer, Brett R. Ullman, Chung-Ming Tse, Zlatina Tarmakova, Cordelia Schiene-Fischer, Gunter Fischer, Imogen Coe, Ville O. Paavilainen, Zhaoli Sun & Jun O. Liu

摘要：Rapamycin and FK506 are macrocyclic natural products with an extraordinary mode of action, in which they form binary complexes with FK506-binding protein (FKBP) through a shared FKBP-binding domain before forming ternary complexes with their respective targets, mechanistic target of rapamycin (mTOR) and calcineurin, respectively. Inspired by this, we sought to build a rapamycin-like macromolecule library to target new cellular proteins by replacing the effector domain of rapamycin with a combinatorial library of oligopeptides. We developed a robust macrocyclization method using ring-closing metathesis and synthesized a 45,000-compound library of hybrid macrocycles (named rapafucins) using optimized FKBP-binding domains. Screening of the rapafucin library in human cells led to the discovery of rapadocin, an inhibitor of nucleoside uptake. Rapadocin is a potent, isoform-specific and FKBP-dependent inhibitor of the equilibrative nucleoside transporter 1 and is efficacious in an animal model of kidney ischaemia reperfusion injury. Together, these results demonstrate that rapafucins are a new class of chemical probes and drug leads that can expand the repertoire of protein targets well beyond mTOR and calcineurin.

链接：https://www.nature.com/articles/s41557-018-0187-4

25. **标题：**Hierarchical organization of perylene bisimides and polyoxometalates for photo-assisted water oxidation

作者：Marcella Bonchio, Zois Syrgiannis, Max Burian, Nadia Marino, Erica Pizzolato, Konstantin Dirian, Francesco Rigodanza, Giulia Alice Volpato, Giuseppina La Ganga, Nicola Demitri, Serena Berardi, Heinz Amenitsch, Dirk M. Guldi, Stefano Caramori, Carlo Alberto Bignozzi, Andrea Sartorel & Maurizio Prato

摘要：The oxygen in Earth’s atmosphere is there primarily because of water oxidation performed by photosynthetic organisms using solar light and one specialized protein complex, photosystem II (PSII). High-resolution imaging of the PSII 'core' complex shows the ideal co-localization of multi-chromophore light-harvesting antennas with the functional reaction centre. Man-made systems are still far from replicating the complexity of PSII, as the majority of PSII mimetics have been limited to photocatalytic dyads based on a 1:1 ratio of a light absorber, generally a Ru–polypyridine complex, with a water oxidation catalyst. Here we report the self-assembly of multi-perylene-bisimide chromophores (PBI) shaped to function by interaction with a polyoxometalate water-oxidation catalyst (Ru4POM). The resulting [PBI]5Ru4POM complex shows a robust amphiphilic structure and dynamic aggregation into large two-dimensional paracrystalline domains, a redshifted light-harvesting efficiency of >40% and favourable exciton accumulation, with a peak quantum efficiency using 'green' photons (λ > 500 nm). The modularity of the building blocks and the simplicity of the non-covalent chemistry offer opportunities for innovation in artificial photosynthesis.

链接：https://www.nature.com/articles/s41557-018-0172-y

IEL Top25

（来源：http://ieeexplore.ieee.org/）

1. 标题：Overview of Dual-Active-Bridge Isolated Bidirectional DC–DC Converter for High-Frequency-Link Power-Conversion System
作者：Biao Zhao ; Qiang Song ; Wenhua Liu ; Yandong Sun
出处：IEEE Transactions on Power Electronics
Volume: 29 Issue: 8 Date : Aug. 2014
Page(s): 4091 - 4106
摘要: High-frequency-link (HFL) power conversion systems (PCSs) are attracting more and more attentions in academia and industry for high power density, reduced weight, and low noise without compromising efficiency, cost, and reliability. In HFL PCSs, dual-active-bridge (DAB) isolated bidirectional dc-dc converter (IBDC) serves as the core circuit. This paper gives an overview of DAB-IBDC for HFL PCSs. First, the research necessity and development history are introduced. Second, the research subjects about basic characterization, control strategy, soft-switching solution and variant, as well as hardware design and optimization are reviewed and analyzed. On this basis, several typical application schemes of DAB-IBDC for HPL PCSs are presented in a worldwide scope. Finally, design recommendations and future trends are presented. As the core circuit of HFL PCSs, DAB-IBDC has wide prospects. The large-scale practical application of DAB-IBDC for HFL PCSs is expected with the recent advances in solid-state semiconductors, magnetic and capacitive materials, and microelectronic technologies.

链接：https://ieeexplore.ieee.org/document/6658916

2.标题：Digital Twin and Big Data Towards Smart Manufacturing and Industry 4.0: 360 Degree Comparison
作者：Qinglin Qi ; Fei Tao
出处：IEEE Access
Volume: 6 Date : 2018
Page(s): 3585 - 3593
摘要: With the advances in new-generation information technologies, especially big data and digital twin, smart manufacturing is becoming the focus of global manufacturing transformation and upgrading. Intelligence comes from data. Integrated analysis for the manufacturing big data is beneficial to all aspects of manufacturing. Besides, the digital twin paves a way for the cyber-physical integration of manufacturing, which is an important bottleneck to achieve smart manufacturing. In this paper, the big data and digital twin in manufacturing are reviewed, including their concept as well as their applications in product design, production planning, manufacturing, and predictive maintenance. On this basis, the similarities and differences between big data and digital twin are compared from the general and data perspectives. Since the big data and digital twin can be complementary, how they can be integrated to promote smart manufacturing are discussed.
链接：https://ieeexplore.ieee.org/document/8258937/

3.标题：Interactive Medical Image Segmentation Using Deep Learning With Image-Specific Fine Tuning
作者：Guotai Wang ; Wenqi Li ; Maria A. Zuluaga ; Rosalind Pratt ; Premal A. Patel ; Michael Aertsen ; Tom Doel ; Anna L. David ; Jan Deprest ; S ébastien Ourselin ; Tom Vercauteren
出处：IEEE Transactions on Medical Imaging
Volume: 37 Issue: 7 Date : July 2018
Page(s): 1562 - 1573
摘要: Convolutional neural networks (CNNs) have achieved state-of-the-art performance for automatic medical image segmentation. However, they have not demonstrated sufficiently accurate and robust results for clinical use. In addition, they are limited by the lack of image-specific adaptation and the lack of generalizability to previously unseen object classes (a.k.a. zero-shot learning). To address these problems, we propose a novel deep learning-based interactive segmentation framework by incorporating CNNs into a bounding box and scribble-based segmentation pipeline. We propose image-specific fine tuning to make a CNN model adaptive to a specific test image, which can be either unsupervised (without additional user interactions) or supervised (with additional scribbles). We also propose a weighted loss function considering network and interaction-based uncertainty for the fine tuning. We applied this framework to two applications: 2-D segmentation of multiple organs from fetal magnetic resonance (MR) slices, where only two types of these organs were annotated for training and 3-D segmentation of brain tumor core (excluding edema) and whole brain tumor (including edema) from different MR sequences, where only the tumor core in one MR sequence was annotated for training. Experimental results show that: 1) our model is more robust to segment previously unseen objects than state-of-the-art CNNs; 2) image-specific fine tuning with the proposed weighted loss function significantly improves segmentation accuracy; and 3) our method leads to accurate results with fewer user interactions and

less user time than traditional interactive segmentation methods.

链接：https://ieeexplore.ieee.org/document/8270673

4.标题：Representation Learning: A Review and New Perspectives
作者：Yoshua Bengio ; Aaron Courville ; Pascal Vincent
出处：IEEE Transactions on Pattern Analysis and Machine Intelligence
Volume: 35 Issue: 8 Date : Aug. 2013
Page(s): 1798 - 1828

摘要: The success of machine learning algorithms generally depends on data representation, and we hypothesize that this is because different representations can entangle and hide more or less the different explanatory factors of variation behind the data. Although specific domain knowledge can be used to help design representations, learning with generic priors can also be used, and the quest for AI is motivating the design of more powerful representation-learning algorithms implementing such priors. This paper reviews recent work in the area of unsupervised feature learning and deep learning, covering advances in probabilistic models, autoencoders, manifold learning, and deep networks. This motivates longer term unanswered questions about the appropriate objectives for learning good representations, for computing representations (i.e., inference), and the geometrical connections between representation learning, density estimation, and manifold learning.

链接：https://ieeexplore.ieee.org/document/6472238

5.标题：Blockchain for AI: Review and Open Research Challenges
作者：Khaled Salah ; M. Habib Ur Rehman ; Nishara Nizamuddin ; Ala Al-Fuqaha
出处：IEEE Access
Volume: 7 Date : 2019
Page(s): 10127 - 10149

摘要：Recently, artificial intelligence (AI) and blockchain have become two of the most trending and disruptive technologies. Blockchain technology has the ability to automate payment in cryptocurrency and to provide access to a shared ledger of data, transactions, and logs in a decentralized, secure, and trusted manner. Also with smart contracts, blockchain has the ability to govern interactions among participants with no intermediary or a trusted third party. AI, on the other hand, offers intelligence and decision-making capabilities for machines similar to humans. In this paper, we present a detailed survey on blockchain applications for AI. We review the literature, tabulate, and summarize the emerging blockchain applications, platforms, and protocols specifically targeting AI area. We also identify and discuss open research challenges of utilizing blockchain technologies for AI.

链接：https://ieeexplore.ieee.org/document/8598784

6.标题：Knowledge Graph Embedding: A Survey of Approaches and Applications
作者：Quan Wang ; Zhendong Mao ; Bin Wang ; Li Guo
出处：IEEE Transactions on Knowledge and Data Engineering
Volume: 29 Issue: 12 Date : 1 Dec. 2017
Page(s): 2724 - 2743

摘要: Knowledge graph (KG) embedding is to embed components of a KG including entities and relations into continuous vector spaces, so as to simplify the manipulation while preserving the inherent structure of the KG. It can benefit a variety of downstream tasks such as KG completion and relation extraction, and hence has quickly gained massive attention. In this article, we provide a systematic review of existing techniques, including not only the state-of-the-arts but also those with latest trends. Particularly, we make the review based on the type of information used in the embedding task. Techniques that conduct embedding using only facts observed in the KG are first introduced. We describe the overall framework, specific model design, typical training procedures, as well as pros and cons of such techniques. After that, we discuss techniques that further incorporate additional information besides facts. We focus specifically on the use of entity types, relation paths, textual descriptions, and logical rules. Finally, we briefly introduce how KG embedding can be applied to and benefit a wide variety of downstream tasks such as KG completion, relation extraction, question answering, and so forth.

链接：https://ieeexplore.ieee.org/document/8047276/

7.标题：Index Modulation Techniques for Next-Generation Wireless Networks

作者：Ertugrul Basar ; Miaowen Wen ; Raed Mesleh ; Marco Di Renzo ; Yue Xiao ; Harald Haas

出处：IEEE Access

Volume: 5 Date : 2017

Page(s): 16693 - 16746

摘要: What is index modulation (IM)? This is an interesting question that we have started to hear more and more frequently over the past few years. The aim of this paper is to answer this question in a comprehensive manner by covering not only the basic principles and emerging variants of IM, but also reviewing the most recent as well as promising advances in this field toward the application scenarios foreseen in next-generation wireless networks. More specifically, we investigate three forms of IM: spatial modulation, channel modulation and orthogonal frequency division multiplexing (OFDM) with IM, which consider the transmit antennas of a multiple-input multiple-output system, the radio frequency mirrors (parasitic elements) mounted at a transmit antenna and the subcarriers of an OFDM system for IM techniques, respectively. We present the up-to-date advances in these three promising frontiers and discuss possible future research directions for IM-based schemes toward low-complexity, spectrum- and energy-efficient next-generation wireless networks.

链接：https://ieeexplore.ieee.org/document/8004416/

8.标题：SoK: Research Perspectives and Challenges for Bitcoin and Cryptocurrencies

作者：Joseph Bonneau ; Andrew Miller ; Jeremy Clark ; Arvind Narayanan ; Joshua A. Kroll ; Edward W. Felten

出处：2015 IEEE Symposium on Security and Privacy

Date : 17-21 May 2015

Page(s): 104 - 121

摘要: Bit coin has emerged as the most successful cryptographic currency in history. Within two years of its quiet launch in 2009, Bit coin grew to comprise billions of dollars of economic value despite only cursory analysis of the system's design. Since then a growing literature has identified hidden-but-important properties of the system, discovered attacks, proposed promising alternatives, and singled out difficult future challenges. Meanwhile a large and vibrant open-source community has proposed and deployed numerous modifications and extensions. We provide the first systematic exposition Bit coin and the many related crypto currencies or 'altcoins.' Drawing from a scattered body of knowledge, we identify three key components of Bit coin's design that can be decoupled. This enables a more insightful analysis of Bit coin's properties and future stability. We map the design space for numerous proposed modifications, providing comparative analyses for alternative consensus mechanisms, currency allocation mechanisms, computational puzzles, and key management tools. We survey anonymity issues in Bit coin and provide an evaluation framework for analyzing a variety of privacy-enhancing proposals. Finally we provide new insights on what we term disinter mediation protocols, which absolve the need for trusted intermediaries in an interesting set of applications. We identify three general disinter mediation strategies and provide a detailed comparison.

链接：https://ieeexplore.ieee.org/document/7163021/

9.标题：Enabling Identity-Based Integrity Auditing and Data Sharing With Sensitive Information Hiding for Secure Cloud Storage

作者：Wenting Shen ; Jing Qin ; Jia Yu ; Rong Hao ; Jiankun Hu

出处：IEEE Transactions on Information Forensics and Security

Volume: 14 Issue: 2 Date : Feb. 2019

Page(s): 331 - 346

摘要：With cloud storage services, users can remotely store their data to the cloud and realize the data sharing with others. Remote data integrity auditing is proposed to guarantee the integrity of the data stored in the cloud. In some common cloud storage systems such as the electronic health records system, the cloud file might contain some sensitive information. The sensitive information should not be exposed to others when the cloud file is shared. Encrypting the whole shared file can realize the sensitive information hiding, but will make this shared file unable to be used by others. How to realize data sharing with sensitive information hiding in remote data integrity auditing still has not been explored up to now. In order to address this problem, we propose a remote data integrity auditing scheme that realizes data sharing with sensitive information hiding in this paper. In this scheme, a sanitizer is used to sanitize the data blocks corresponding to the sensitive information of the file and transforms these data blocks' signatures into valid ones for the sanitized file. These signatures are used to verify the integrity of the sanitized file in the phase of integrity auditing. As a result, our scheme makes the file stored in the cloud able to be shared and used by others on the condition that the sensitive information is hidden, while the remote data integrity auditing is still able to be efficiently executed. Meanwhile, the proposed scheme is based on identity-based cryptography, which simplifies the complicated certificate management. The security analysis and the performance evaluation show that the proposed scheme is secure and efficient.

链接：https://ieeexplore.ieee.org/document/8395433/

10.标题：Software-Defined Networking: A Comprehensive Survey

作者：Diego Kreutz ; Fernando M. V. Ramos ; Paulo Esteves Ver ́ssimo ; Christian Esteve Rothenberg ; Siamak Azodolmolky ; Steve Uhlig

出处：Proceedings of the IEEE

Volume: 103 Issue: 1 Date : Jan. 2015

Page(s): 14 - 76

摘要: The Internet has led to the creation of a digital society, where (almost) everything is connected and is accessible from anywhere. However, despite their widespread adoption, traditional IP

networks are complex and very hard to manage. It is both difficult to configure the network according to predefined policies, and to reconfigure it to respond to faults, load, and changes. To make matters even more difficult, current networks are also vertically integrated: the control and data planes are bundled together. Software-defined networking (SDN) is an emerging paradigm that promises to change this state of affairs, by breaking vertical integration, separating the network's control logic from the underlying routers and switches, promoting (logical) centralization of network control, and introducing the ability to program the network. The separation of concerns, introduced between the definition of network policies, their implementation in switching hardware, and the forwarding of traffic, is key to the desired flexibility: by breaking the network control problem into tractable pieces, SDN makes it easier to create and introduce new abstractions in networking, simplifying network management and facilitating network evolution. In this paper, we present a comprehensive survey on SDN. We start by introducing the motivation for SDN, explain its main concepts and how it differs from traditional networking, its roots, and the standardization activities regarding this novel paradigm. Next, we present the key building blocks of an SDN infrastructure using a bottom-up, layered approach. We provide an in-depth analysis of the hardware infrastructure, southbound and northbound application programming interfaces (APIs), network virtualization layers, network operating systems (SDN controllers), network programming languages, and network applications. We also look at cross-layer problems such as debugging and troubleshooting. In an effort to anticipate the future evolution of this ne...
链接：https://ieeexplore.ieee.org/document/6994333

11.标题：A Tutorial on IEEE 802.11ax High Efficiency WLANs
作者：Evgeny Khorov ; Anton Kiryanov ; Andrey Lyakhov ; Giuseppe Bianchi
出处：IEEE Communications Surveys & Tutorials
Volume: 21 Issue: 1 Date : Firstquarter 2019
Page(s): 197 - 216
摘要: While celebrating the 21st year since the very first IEEE 802.11 “legacy” 2 Mbit/s wireless local area network standard, the latest Wi-Fi newborn is today reaching the finish line, topping the remarkable speed of 10 Gbit/s. IEEE 802.11ax was launched in May 2014 with the goal of enhancing throughput-per-area in high-density scenarios. The first 802.11ax draft versions, namely, D1.0 and D2.0, were released at the end of 2016 and 2017. Focusing on a more mature version D3.0, in this tutorial paper, we help the reader to smoothly enter into the several major 802.11ax breakthroughs, including a brand new orthogonal frequency-division multiple access-based random access approach as well as novel spatial frequency reuse techniques. In addition, this tutorial will highlight selected significant improvements (including physical layer enhancements, multi-user multiple input multiple output extensions, power saving advances, and so on) which make this standard a very significant step forward with respect to its predecessor 802.11ac.
链接：https://ieeexplore.ieee.org/document/8468986/

12.标题：When Intrusion Detection Meets Blockchain Technology: A Review
作者：Weizhi Meng ; Elmar Wolfgang Tischhauser ; Qingju Wang ; Yu Wang ; Jinguang Han
出处：IEEE Access
Volume: 6 Date : 2018
Page(s): 10179 - 10188

摘要: With the purpose of identifying cyber threats and possible incidents, intrusion detection systems (IDSs) are widely deployed in various computer networks. In order to enhance the detection capability of a single IDS, collaborative intrusion detection networks (or collaborative IDSs) have been developed, which allow IDS nodes to exchange data with each other. However, data and trust management still remain two challenges for current detection architectures, which may degrade the effectiveness of such detection systems. In recent years, blockchain technology has shown its adaptability in many fields, such as supply chain management, international payment, interbanking, and so on. As blockchain can protect the integrity of data storage and ensure process transparency, it has a potential to be applied to intrusion detection domain. Motivated by this, this paper provides a review regarding the intersection of IDSs and blockchains. In particular, we introduce the background of intrusion detection and blockchain, discuss the applicability of blockchain to intrusion detection, and identify open challenges in this direction.

链接：https://ieeexplore.ieee.org/document/8274922/

13.标题：Privacy-Preserving Data Mining: Methods, Metrics, and Applications
作者：Ricardo Mendes ; João P. Vilela
出处：IEEE Access
Volume: 5 Date : 2017
Page(s): 10562 - 10582

摘要: The collection and analysis of data are continuously growing due to the pervasiveness of computing devices. The analysis of such information is fostering businesses and contributing beneficially to the society in many different fields. However, this storage and flow of possibly sensitive data poses serious privacy concerns. Methods that allow the knowledge extraction from data, while preserving privacy, are known as privacy-preserving data mining (PPDM) techniques. This paper surveys the most relevant PPDM techniques from the literature and the metrics used to evaluate such techniques and presents typical applications of PPDM methods in relevant fields. Furthermore, the current challenges and open issues in PPDM are discussed.

链接：https://ieeexplore.ieee.org/document/7950921/

14.标题：Wind Energy Systems
作者：Frede Blaabjerg ; Ke Ma
出处：Proceedings of the IEEE
Volume: 105 Issue: 11 Date : Nov. 2017
Page(s): 2116 - 2131

摘要: Wind power now represents a major and growing source of renewable energy. Large wind turbines (with capacities of up to 6-8 MW) are widely installed in power distribution networks. Increasing numbers of onshore and offshore wind farms, acting as power plants, are connected directly to power transmission networks at the scale of hundreds of megawatts. As its level of grid penetration has begun to increase dramatically, wind power is starting to have a significant impact on the operation of the modern grid system. Advanced power electronics technologies are being introduced to improve the characteristics of the wind turbines, and make them more suitable for integration into the power grid. Meanwhile, there are some emerging challenges that still need to be addressed. This paper provides an overview and discusses some trends in the power electronics technologies used for wind power generation. First, the state-of-the-art technology and global market are generally discussed. Several important wind turbine concepts are discussed, along with power electronics solutions either for individual wind turbines or for entire wind farms. Some technology challenges and future solutions for power electronics in wind turbine systems are also addressed.

链接：https://ieeexplore.ieee.org/document/7927779

15.标题：Image quality assessment: from error visibility to structural similarity
作者：Zhou Wang ; A.C. Bovik ; H.R. Sheikh ; E.P. Simoncelli
出处：IEEE Transactions on Image Processing
Volume: 13 Issue: 4 Date : April 2004
Page(s): 600 - 612

摘要: Objective methods for assessing perceptual image quality traditionally attempted to quantify the visibility of errors (differences) between a distorted image and a reference image using a variety of known properties of the human visual system. Under the assumption that human visual perception is highly adapted for extracting structural information from a scene, we introduce an alternative complementary framework for quality assessment based on the degradation of structural information. As a specific example of this concept, we develop a structural similarity index and demonstrate its promise through a set of intuitive examples, as well as comparison to both subjective ratings and state-of-the-art objective methods on a database of images compressed with JPEG and JPEG2000. A MATLAB implementation of the proposed algorithm is available online at http://www.cns.nyu.edu//spl sim/lcv/ssim/.

链接：https://ieeexplore.ieee.org/document/1284395/

16.标题：Traffic Flow Prediction With Big Data: A Deep Learning Approach
作者：Yisheng Lv ; Yanjie Duan ; Wenwen Kang ; Zhengxi Li ; Fei-Yue Wang
出处：IEEE Transactions on Intelligent Transportation Systems
Volume: 16 Issue: 2 Date : April 2015
Page(s): 865 - 873

摘要: Accurate and timely traffic flow information is important for the successful deployment of intelligent transportation systems. Over the last few years, traffic data have been exploding, and we have truly entered the era of big data for transportation. Existing traffic flow prediction methods mainly use shallow traffic prediction models and are still unsatisfying for many real-world applications. This situation inspires us to rethink the traffic flow prediction problem based on deep architecture models with big traffic data. In this paper, a novel deep-learning-based traffic flow prediction method is proposed, which considers the spatial and temporal correlations inherently. A stacked autoencoder model is used to learn generic traffic flow features, and it is trained in a greedy layerwise fashion. To the best of our knowledge, this is the first time that a deep architecture model is applied using autoencoders as building blocks to represent traffic flow features for prediction. Moreover, experiments demonstrate that the proposed method for traffic flow prediction has superior performance.

链接： https://ieeexplore.ieee.org/document/6894591

17.标题：Tensor Decomposition for Signal Processing and Machine Learning
作者：Nicholas D. Sidiropoulos ; Lieven De Lathauwer ; Xiao Fu ; Kejun Huang ; Evangelos E. Papalexakis ; Christos Faloutsos

出处：IEEE Transactions on Signal Processing
Volume: 65 Issue: 13 Date : 1 July1, 2017
Page(s): 3551 - 3582
摘要: Tensors or multiway arrays are functions of three or more indices (i, j, k, . . .)-similar to matrices (two-way arrays), which are functions of two indices (r, c) for (row, column). Tensors have a rich history, stretching over almost a century, and touching upon numerous disciplines; but they have only recently become ubiquitous in signal and data analytics at the confluence of signal processing, statistics, data mining, and machine learning. This overview article aims to provide a good starting point for researchers and practitioners interested in learning about and working with tensors. As such, it focuses on fundamentals and motivation (using various application examples), aiming to strike an appropriate balance of breadth and depth that will enable someone having taken first graduate courses in matrix algebra and probability to get started doing research and/or developing tensor algorithms and software. Some background in applied optimization is useful but not strictly required. The material covered includes tensor rank and rank decomposition; basic tensor factorization models and their relationships and properties (including fairly good coverage of identifiability); broad coverage of algorithms ranging from alternating optimization to stochastic gradient; statistical performance analysis; and applications ranging from source separation to collaborative filtering, mixture and topic modeling, classification, and multilinear subspace learning.
链接：https://ieeexplore.ieee.org/document/7891546

18.标题：Faster R-CNN: Towards Real-Time Object Detection with Region Proposal Networks
作者：Shaoqing Ren ; Kaiming He ; Ross Girshick ; Jian Sun
出处：IEEE Transactions on Pattern Analysis and Machine Intelligence
Volume: 39 Issue: 6 Date : 1 June 2017
Page(s): 1137 - 1149
摘要: State-of-the-art object detection networks depend on region proposal algorithms to hypothesize object locations. Advances like SPPnet [1] and Fast R-CNN [2] have reduced the running time of these detection networks, exposing region proposal computation as a bottleneck. In this work, we introduce a Region Proposal Network(RPN) that shares full-image convolutional features with the detection network, thus enabling nearly cost-free region proposals. An RPN is a fully convolutional network that simultaneously predicts object bounds and objectness scores at each position. The RPN is trained end-to-end to generate high-quality region proposals, which are used by Fast R-CNN for detection. We further merge RPN and Fast R-CNN into a single network by sharing their convolutional features-using the recently popular terminology of neural networks with 'attention' mechanisms, the RPN component tells the unified network where to look. For the very deep VGG-16 model [3], our detection system has a frame rate of 5 fps (including all steps) on a GPU, while achieving state-of-the-art object detection accuracy on PASCAL VOC 2007, 2012, and MS COCO datasets with only 300 proposals per image. In ILSVRC and COCO 2015 competitions, Faster R-CNN and RPN are the foundations of the 1st-place winning entries in several tracks. Code has been made publicly available.
链接：https://ieeexplore.ieee.org/document/7485869

19.标题：Action Recognition in Video Sequences using Deep Bi-Directional LSTM With CNN Features
作者：Amin Ullah ; Jamil Ahmad ; Khan Muhammad ; Muhammad Sajjad ; Sung Wook Baik
出处：IEEE Access
Volume: 6 Date : 2018
Page(s): 1155 - 1166

摘要：Cloud computing with its three key facets (i.e., Infrastructure-as-a-Service, Platform-as-a-Service, and Software-as-a-Service) and its inherent advantages (e.g., elasticity and scalability) still faces several challenges. The distance between the cloud and the end devices might be an issue for latency-sensitive applications such as disaster management and content delivery applications. Service level agreements (SLAs) may also impose processing at locations where the cloud provider does not have data centers. Fog computing is a novel paradigm to address such issues. It enables provisioning resources and services outside the cloud, at the edge of the network, closer to end devices, or eventually, at locations stipulated by SLAs. Fog computing is not a substitute for cloud computing but a powerful complement. It enables processing at the edge while still offering the possibility to interact with the cloud. This paper presents a comprehensive survey on fog computing. It critically reviews the state of the art in the light of a concise set of evaluation criteria. We cover both the architectures and the algorithms that make fog systems. Challenges and research directions are also introduced. In addition, the lessons learned are reviewed and the prospects are discussed in terms of the key role fog is likely to play in emerging technologies such as tactile Internet.

链接：https://ieeexplore.ieee.org/document/8100873

20.标题：A Comprehensive Survey on Fog Computing: State-of-the-Art and Research Challenges
作者：Carla Mouradian ; Diala Naboulsi ; Sami Yangui ; Roch H. Glitho ; Monique J. Morrow ; Paul A. Polakos
出处：IEEE Communications Surveys & Tutorials
Volume: 20 Issue: 1 Date : Firstquarter 2018
Page(s): 416 - 464

摘要：Cloud computing with its three key facets (i.e., Infrastructure-as-a-Service, Platform-as-a-Service, and Software-as-a-Service) and its inherent advantages (e.g., elasticity and scalability) still faces several challenges. The distance between the cloud and the end devices might be an issue for latency-sensitive applications such as disaster management and content delivery applications. Service level agreements (SLAs) may also impose processing at locations where the cloud provider does not have data centers. Fog computing is a novel paradigm to address such issues. It enables provisioning resources and services outside the cloud, at the edge of the network, closer to end devices, or eventually, at locations stipulated by SLAs. Fog computing is not a substitute for cloud computing but a powerful complement. It enables processing at the edge while still offering the possibility to interact with the cloud. This paper presents a comprehensive survey on fog computing. It critically reviews the state of the art in the light of a concise set of evaluation criteria. We cover both the architectures and the algorithms that make fog systems. Challenges and research directions are also introduced. In addition, the lessons learned are reviewed and the prospects are discussed in terms of the key role fog is likely to play in emerging technologies such as tactile Internet.

链接：https://ieeexplore.ieee.org/document/8100873/

21.标题：Fog and IoT: An Overview of Research Opportunities
作者：Mung Chiang ; Tao Zhang
出处：IEEE Internet of Things Journal
Volume: 3 Issue: 6 Date : Dec. 2016
Page(s): 854 - 864

摘要: Fog is an emergent architecture for computing, storage, control, and networking that distributes these services closer to end users along the cloud-to-things continuum. It covers both mobile and wireline scenarios, traverses across hardware and software, resides on network edge but also over access networks and among end users, and includes both data plane and control plane. As an architecture, it supports a growing variety of applications, including those in the Internet of Things (IoT), fifth-generation (5G) wireless systems, and embedded artificial intelligence (AI). This survey paper summarizes the opportunities and challenges of fog, focusing primarily in the networking context of IoT.

链接：https://ieeexplore.ieee.org/document/7498684

22.标题：A Particle Swarm Optimized Learning Model of Fault Classification in Web-Apps
作者：Deepak Kumar Jain ; Akshi Kumar ; Saurabh Raj Sangwan ; Gia Nhu Nguyen ; Prayag Tiwari
出处：IEEE Access
Volume: 7 Date : 2019
Page(s): 18480 - 18489

摘要：The term web-app defines the current dynamic pragmatics of the website, where the user has control. Finding faults in such dynamic content is challenging, as to whether the fault is exposed or not depends on its execution path. Moreover, the complexity and uniqueness of each web application make fault assessment an extremely laborious and expensive task. Also, artificial fault injection models are run in controlled and simulated environments, which may not be representative of the real-world fault data. Classifying faults can intelligently enhance the quality of the web-apps by the assessment of probable faults. In this paper, an empirical study is conducted to classify faults in bug reports of three open-source web-apps (qaManager, bitWeaver, and WebCalendar) and reviews of two play store web-apps (Dineout: Reserve a Table and Wynk Music). Five supervised learning algorithms (naïve Bayesian, decision tree, support vector machines, K-nearest neighbor, and multi-layer perceptron) have been first evaluated based on the conventional term frequency-inverse document frequency (tf-idf) feature extraction method, and subsequently, a feature selection method to improve classifier performance is proposed using particle swarm optimization (a nature-inspired, meta-heuristic algorithm). This paper is a preliminary exploratory study to build an automated tool, which can optimally categorize faults. The empirical analysis validates that the particle swarm optimization for feature selection in fault classification task outperforms the tf-idf filter-based classifiers with an average accuracy gain of about 11% and nearly 26% average feature reduction. The highest accuracy of 93.35% is shown by the decision tree after feature selection.

链接：https://ieeexplore.ieee.org/document/8639005

23.标题：Blockchain: A game changer for securing IoT data
作者：Madhusudan Singh ; Abhiraj Singh ; Shiho Kim
出处：2018 IEEE 4th World Forum on Internet of Things (WF-IoT)
Date : 5-8 Feb. 2018

Page(s): 51 - 55

摘要: Internet of Things (IoT) is now in its initial stage but very soon, it is going to influence almost every day-to-day items we use. The more it will be included in our lifestyle, more will be the threat of it being misused. There is an urgent need to make IoT devices secure from getting cracked. Very soon IoT is going to expand the area for the cyber-attacks on homes and businesses by transforming objects that were used to be offline into online systems. Existing security technologies are just not enough to deal with this problem. Blockchain has emerged as the possible solution for creating more secure IoT systems in the time to come. In this paper, first an overview of the blockchain technology and its implementation has been explained; then we have discussed the infrastructure of IoT which is based on Blockchain network and at last a model has been provided for the security of internet of things using blockchain.

链接：https://ieeexplore.ieee.org/document/8355182

24.标题：A High Performance Blockchain Platform for Intelligent Devices

作者：Shitang Yu ; Kun Lv ; Zhou Shao ; Yingcheng Guo ; Jun Zou ; Bo Zhang

出处：2018 1st IEEE International Conference on Hot Information-Centric Networking (HotICN)

Date : 15-17 Aug. 2018

Page(s): 260 - 261

摘要: In the area of IoT (Internet of Things), more and more intelligent devices are being connected to the Internet. These intelligent devices have been producing a huge amout of useful data over time, however there is still a lack of a platform which can efficiently transfer and utilize the value of the massive IoT data. Blockchain is able to transfer value with a relative low cost, which makes it possible for the data from smart devices to create economic value. This work of this paper is to design a high performance blockchain platform, using technologies such as distributed network architecture, intelligent devices node mapping, as well as PBFT-DPOC consensus algorithm to realize the decentralized autonomy of intelligent devices.

链接：https://ieeexplore.ieee.org/document/8606017

25.标题：Beyond a Gaussian Denoiser: Residual Learning of Deep CNN for Image Denoising

作者：Kai Zhang ; Wangmeng Zuo ; Yunjin Chen ; Deyu Meng ; Lei Zhang

出处：IEEE Transactions on Image Processing

Volume: 26 Issue: 7 Date : July 2017

Page(s): 3142 - 3155

摘要: The discriminative model learning for image denoising has been recently attracting considerable attentions due to its favorable denoising performance. In this paper, we take one step forward by investigating the construction of feed-forward denoising convolutional neural networks (DnCNNs) to embrace the progress in very deep architecture, learning algorithm, and regularization method into image denoising. Specifically, residual learning and batch normalization are utilized to speed up the training process as well as boost the denoising performance. Different from the existing discriminative denoising models which usually train a specific model for additive white Gaussian noise at a certain noise level, our DnCNN model is able to handle Gaussian denoising with unknown noise level (i.e., blind Gaussian denoising). With the residual learning strategy, DnCNN implicitly removes the latent clean image in the hidden layers. This property motivates us to train a single DnCNN model to tackle with several general image denoising tasks, such as Gaussian denoising, single image super-resolution, and JPEG image deblocking. Our extensive experiments demonstrate that our DnCNN model can not only exhibit high effectiveness in several general image denoising tasks, but also be efficiently implemented by benefiting from GPU computing.

链接：https://ieeexplore.ieee.org/document/7839189

ESI HOT PAPERS

(Chemistry)

（来源：http://esi.incites.thomsonreuters.com）

1.被引频次：1261

题目：IODIDE MANAGEMENT IN FORMAMIDINIUM-LEAD-HALIDE-BASED PEROVSKITE LAYERS FOR EFFICIENT SOLAR CELLS

作者：YANG, WS;PARK, BW;JUNG, EH;JEON, NJ;KIM, YC;LEE, DU;SHIN, SS;SEO, J;KIM, EK;NOH, JH;SEOK, SI

出处：SCIENCE 356 (6345): 1376-+ JUN 30 2017

地址：ULSAN NATL INST SCI & TECHNOL, SCH NAT SCI, PEROVTRON RES CTR, 50 UNIST GIL, ULSAN 44919, SOUTH KOREA;ULSAN NATL INST SCI & TECHNOL, SCH ENERGY & CHEM ENGN, 50 UNIST GIL, ULSAN 44919, SOUTH KOREA;KOREA RES INST CHEM TECHNOL, DIV ADV MAT, 141 GAJEONG RO, DAEJEON 34114, SOUTH KOREA;SK HYNIX INC, NAND PROD ENGN GRP, ICHEON 17336, SOUTH KOREA;HANYANG UNIV, DEPT PHYS, SEOUL 04763, SOUTH KOREA;HANYANG UNIV, QUANTUM FUNCT RES LAB, SEOUL 04763, SOUTH KOREA;KOREA UNIV, SCH CIVIL ENVIRONM & ARCHITECTURAL ENGN, SEOUL 136713, SOUTH KOREA

摘要：The formation of a dense and uniform thin layer on the substrates is crucial for the fabrication of high-performance perovskite solar cells (PSCs) containing formamidinium with multiple cations and mixed halide anions. The concentration of defect states, which reduce a cell's performance by decreasing the open-circuit voltage and short-circuit current density, needs to be as low as possible. We show that the introduction of additional iodide ions into the organic cation solution, which are used to form the perovskite layers through an intramolecular exchanging process, decreases the concentration of deep-level defects. The defect-engineered thin perovskite layers enable the fabrication of PSCs with a certified power conversion efficiency of 22.1% in small cells and 19.7% in 1-square-centimeter cells.

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2.被引频次：735

题目：MOLECULAR OPTIMIZATION ENABLES OVER 13% EFFICIENCY IN ORGANIC SOLAR CELLS

作者：ZHAO, WC;LI, SS;YAO, HF;ZHANG, SQ;ZHANG, Y;YANG, B;HOU, JH

出处：J AM CHEM SOC 139 (21): 7148-7151 MAY 31 2017

地址：CHINESE ACAD SCI, BEIJING NATL LAB MOL SCI, CAS RES EDUCAT CTR EXCELLENCE MOL SCI, STATE KEY LAB POLYMER PHYS & CHEM,INST CHEM, BEIJING 100190, PEOPLES R CHINA;UNIV CHINESE ACAD SCI, BEIJING 100049, PEOPLES R CHINA

摘要：A new polymer donor (PBDB-T-SF) and a new small molecule acceptor (IT-4F) for fullerene-free organic solar cells (OSCs) were designed and synthesized. The influences of fluorination on the absorption spectra, molecular energy levels, and charge mobilities of the donor and acceptor were systematically studied. The PBDB-T-SF:IT-4F-based OSC device showed a record high efficiency of 13.1%, and an efficiency of over 12% can be obtained with a thickness of 100-200 nm, suggesting the promise of fullerene-free OSCs in practical applications.

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3.被引频次：640

题目：COMBINING THEORY AND EXPERIMENT IN ELECTROCATALYSIS: INSIGHTS INTO MATERIALS DESIGN

作者：SEH, ZW;KIBSGAARD, J;DICKENS, CF;CHORKENDORFF, IB;NORSKOV, JK;JARAMILLO, TF

出处：SCIENCE 355 (6321): - JAN 13 2017

地址：STANFORD UNIV, DEPT CHEM ENGN, SUNCAT CTR INTERFACE SCI & CATALYSIS, STANFORD, CA 94305 USA;SLAC NATL ACCELERATOR LAB, SUNCAT CTR INTERFACE SCI & CATALYSIS, MENLO PK, CA 94025 USA;ASTAR, INST MAT RES & ENGN, INNOVIS 138634, SINGAPORE;TECH UNIV DENMARK, DEPT PHYS, DK-2800 LYNGBY, DENMARK

摘要：Electrocatalysis plays a central role in clean energy conversion, enabling a number of sustainable processes for future technologies. This review discusses design strategies for state-of-the-art heterogeneous electrocatalysts and associated materials for several different electrochemical transformations involving water, hydrogen, and oxygen, using theory as a means to rationalize catalyst performance. By examining the common principles that govern catalysis for different electrochemical reactions, we describe a systematic framework that clarifies trends in catalyzing these reactions, serving as a guide to new catalyst development while highlighting key gaps that need to be addressed. We conclude by extending this framework to emerging clean energy reactions such as hydrogen peroxide production, carbon dioxide reduction, and nitrogen reduction, where the development of improved catalysts could allow for the sustainable production of a broad range of fuels and chemicals.

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4.被引频次：535

题目：RECENT ADVANCES IN ULTRATHIN TWO-DIMENSIONAL NANOMATERIALS

作者：TAN, CL;CAO, XH;WU, XJ;HE, QY;YANG, J;ZHANG, X;CHEN, JZ;ZHAO, W;HAN, SK;NAM, GH;SINDORO, M;ZHANG, H

出处：CHEM REV 117 (9): 6225-6331 MAY 10 2017

地址：NANYANG TECHNOL UNIV, SCH MAT SCI & ENGN, CTR PROGRAMMABLE MAT, 50 NANYANG AVE, SINGAPORE 639798, SINGAPORE;ZHEJIANG UNIV TECHNOL, COLL MAT SCI & ENGN, 18 CHAOWANG RD, HANGZHOU 310014, ZHEJIANG, PEOPLES R CHINA

摘要：Since the discovery of mechanically exfoliated graphene in 2004, research on ultrathin two-dimensional (2D) nanomaterials has grown exponentially in the fields of condensed matter physics, material science, chemistry, and nanotechnology. Highlighting their compelling physical, chemical, electronic, and optical properties, as well as their various potential applications, in this Review, we summarize the state-of-art progress on the ultrathin 2D nanomaterials with a particular emphasis on their recent advances. First, we introduce the unique advances on ultrathin 2D nanomaterials, followed by the description of their composition and crystal structures. The assortments of their synthetic methods are then summarized, including insights on their advantages and limitations, alongside some recommendations on suitable characterization techniques. We also discuss in detail the utilization of these ultrathin 2D nanomaterials for wide ranges of potential applications among the electronics/optoelectronics, electrocatalysis, batteries, supercapacitors, solar cells, photo catalysis, and sensing platforms. Finally, the challenges and outlooks in this promising field are featured on the basis of its current development.

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5.被引频次：451

题目：EFFICIENT AND STABLE SOLUTION-PROCESSED PLANAR PEROVSKITE SOLAR CELLS VIA CONTACT PASSIVATION

作者：TAN, HR;JAIN, A;VOZNYY, O;LAN, XZ;DE ARQUER, FPG;FAN, JZ;QUINTERO-BERMUDEZ, R;YUAN, MJ;ZHANG, B;ZHAO, YC;FAN, FJ;LI, PC;QUAN, LN;ZHAO, YB;LU, ZH;YANG, ZY;HOOGLAND, S;SARGENT, EH

出处：SCIENCE 355 (6326): 722-726 FEB 17 2017

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摘要：Planar perovskite solar cells (PSCs) made entirely via solution processing at low temperatures (<150 degrees C) offer promise for simple manufacturing, compatibility with flexible substrates, and perovskite-based tandem devices. However, these PSCs require an electron-selective layer that performs well with similar processing. We report a contact-passivation strategy using chlorine-capped TiO2 colloidal nanocrystal film that mitigates interfacial recombination and improves interface binding in low-temperature planar solar cells. We fabricated solar cells with certified efficiencies of 20.1 and 19.5% for active areas of 0.049 and 1.1 square centimeters, respectively, achieved via low-temperature solution processing. Solar cells with efficiency greater than 20% retained 90% (97% after dark recovery) of their initial performance after 500 hours of continuous room-temperature operation at their maximum power point under 1-sun illumination (where 1 sun is defined as the standard illumination at AM1.5, or 1 kilowatt/square meter).

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6.被引频次：412
题目：ELECTROCATALYSIS FOR THE OXYGEN EVOLUTION REACTION: RECENT DEVELOPMENT AND FUTURE PERSPECTIVES
作者：SUEN, NT;HUNG, SF;QUAN, Q;ZHANG, N;XU, YJ;CHEN, HM
出处：CHEM SOC REV 46 (2): 337-365 JAN 21 2017
地址：NATL TAIWAN UNIV, DEPT CHEM, 1,SEC 4,ROOSEVELT RD, TAIPEI 10617, TAIWAN;FUZHOU UNIV, COLL CHEM, STATE KEY LAB PHOTOCATALYSIS ENERGY & ENVIRONM, FUZHOU 350002, PEOPLES R CHINA
摘要：There is still an ongoing effort to search for sustainable, clean and highly efficient energy generation to satisfy the energy needs of modern society. Among various advanced technologies, electrocatalysis for the oxygen evolution reaction (OER) plays a key role and numerous new electrocatalysts have been developed to improve the efficiency of gas evolution. Along the way, enormous effort has been devoted to finding high-performance electrocatalysts, which has also stimulated the invention of new techniques to investigate the properties of materials or the fundamental mechanism of the OER. This accumulated knowledge not only establishes the foundation of the mechanism of the OER, but also points out the important criteria for a good electrocatalyst based on a variety of studies. Even though it may be difficult to include all cases, the aim of this review is to inspect the current progress and offer a comprehensive insight toward the OER. This review begins with examining the theoretical principles of electrode kinetics and some measurement criteria for achieving a fair evaluation among the catalysts. The second part of this review acquaints some materials for performing OER activity, in which the metal oxide materials build the basis of OER mechanism white non-oxide materials exhibit greatly promising performance toward overall water-splitting. Attention of this review is also paid to in situ approaches to electrocatalytic behavior during OER, and this information is crucial and can provide efficient strategies to design perfect electrocatalysts for OER. Finally, the OER mechanism from the perspective of both recent experimental and theoretical investigations is discussed, as well as probable strategies for improving OER performance with regards to future developments.
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7.被引频次：350
题目：METAL-ORGANIC FRAMEWORKS: FUNCTIONAL LUMINESCENT AND PHOTONIC MATERIALS FOR SENSING APPLICATIONS
作者：LUSTIG, WP;MUKHERJEE, S;RUDD, ND;DESAI, AV;LI, J;GHOSH, SK
出处：CHEM SOC REV 46 (11): 3242-3285 JUN 7 2017
地址：RUTGERS STATE UNIV, DEPT CHEM & CHEM BIOL, PISCATAWAY, NJ 08854 USA;INDIAN INST SCI EDUC & RES, DR HOMI BHABHA RD, PUNE 411008, MAHARASHTRA, INDIA
摘要：Metal-organic frameworks (MOFs) or porous coordination polymers (PCPs) are open, crystalline supra-molecular coordination architectures with porous facets. These chemically tailorable framework materials are the subject of intense and expansive research, and are particularly relevant in the fields of sensory materials and device engineering. As the subfield of MOF-based sensing has developed, many diverse chemical functionalities have been carefully and rationally implanted into the coordination nanospace of MOF materials. MOFs with widely varied fluorometric sensing properties have been developed using the design principles of crystal engineering and

structure-property correlations, resulting in a large and rapidly growing body of literature. This work has led to advancements in a number of crucial sensing domains, including biomolecules, environmental toxins, explosives, ionic species, and many others. Furthermore, new classes of MOF sensory materials utilizing advanced signal transduction by devices based on MOF photonic crystals and thin films have been developed. This comprehensive review summarizes the topical developments in the field of luminescent MOF and MOF-based photonic crystals/thin film sensory materials.
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8.被引频次：334
题目：MULTIFUNCTIONAL METAL-ORGANIC FRAMEWORK CATALYSTS: SYNERGISTIC CATALYSIS AND TANDEM REACTIONS
作者：HUANG, YB;LIANG, J;WANG, XS;CAO, R
出处：CHEM SOC REV 46 (1): 126-157 JAN 7 2017
地址：CHINESE ACAD SCI, FUJIAN INST RES STRUCT MATTER, STATE KEY LAB STRUCT CHEM, FUZHOU 350002, FUJIAN, PEOPLES R CHINA
摘要：Metal-organic frameworks (MOFs) are porous crystalline materials constructed from metal ions or clusters and multidentate organic ligands. Recently, the use of MOFs or MOF composites as catalysts for synergistic catalysis and tandem reactions has attracted increasing attention due to their tunable open metal centres, functional organic linkers, and active guest species in their pores. In this review, the applications of MOFs with multiple active sites in synergistic organic catalysis, photocatalysis and tandem reactions are discussed. These multifunctional MOFs can be categorized by the type of active centre as follows: (i) open metal centres and functional organic linkers in the MOF structure, (ii) active guest sites in the pores and active sites in the MOF structure, and (iii) bimetallic nanoparticles (NPs) on MOF supports. The types of synergistic catalysis and tandem reactions promoted by multifunctional MOFs and their proposed mechanisms are presented in detail. Here, catalytic MOFs with a single type of active site and MOFs that only serve as supports to enhance substrate adsorption are not discussed.
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9.被引频次：334
题目：SODIUM-ION BATTERIES: PRESENT AND FUTURE
作者：HWANG, JY;MYUNG, ST;SUN, YK
出处：CHEM SOC REV 46 (12): 3529-3614 JUN 21 2017
地址：HANYANG UNIV, DEPT ENERGY ENGN, SEOUL 04763, SOUTH KOREA;SEJONG UNIV, DEPT NANOTECHNOL & ADV MAT ENGN, SEOUL 05006, SOUTH KOREA
摘要：Energy production and storage technologies have attracted a great deal of attention for day-to-day applications. In recent decades, advances in lithium-ion battery (LIB) technology have improved living conditions around the globe. LIBs are used in most mobile electronic devices as well as in zero-emission electronic vehicles. However, there are increasing concerns regarding load leveling of renewable energy sources and the smart grid as well as the sustainability of lithium sources due to their limited availability and consequent expected price increase. Therefore, whether LIBs alone can satisfy the rising demand for small-and/or mid-to-large-format energy storage applications remains unclear. To mitigate these issues, recent research has focused on alternative

energy storage systems. Sodium-ion batteries (SIBs) are considered as the best candidate power sources because sodium is widely available and exhibits similar chemistry to that of LIBs; therefore, SIBs are promising next-generation alternatives. Recently, sodiated layer transition metal oxides, phosphates and organic compounds have been introduced as cathode materials for SIBs. Simultaneously, recent developments have been facilitated by the use of select carbonaceous materials, transition metal oxides (or sulfides), and intermetallic and organic compounds as anodes for SIBs. Apart from electrode materials, suitable electrolytes, additives, and binders are equally important for the development of practical SIBs. Despite developments in electrode materials and other components, there remain several challenges, including cell design and electrode balancing, in the application of sodium ion cells. In this article, we summarize and discuss current research on materials and propose future directions for SIBs. This will provide important insights into scientific and practical issues in the development of SIBs.
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10.被引频次：333
题目：PALLADIUM-CATALYZED TRANSFORMATIONS OF ALKYL C-H BONDS
作者：HE, J;WASA, M;CHAN, KSL;SHAO, O;YU, JQ
出处：CHEM REV 117 (13): 8754-8786 JUL 12 2017
地址：SCRIPPS RES INST, DEPT CHEM, 10550 N TORREY PINES RD, LA JOLLA, CA 92037 USA
摘要：This Review summarizes the advancements in Pd-catalyzed C(sp(3))-H activation via various redox manifolds, including Pd(0)/Pd(II), Pd(II)/Pd(W), and Pd(II)/Pd(0). While few examples have been reported in the activation of alkane C -H bonds, many C(sp(3))-H activation/C-C and C-heteroatom bond forming reactions have been developed by the use of directing group strategies to control regioselectivity and build structural patterns for synthetic chemistry. A number of mono- and bidentate ligands have also proven to be effective for accelerating C(sp(3))-H activation, directed by weakly coordinating auxiliaries, which provides great opportunities to control reactivity and selectivity (including enantioselectivity) in Pd-catalyzed C-H functionalization reactions.
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11.被引频次：325
题目：TRANSITION METAL-CATALYZED C-H AMINATION: SCOPE, MECHANISM, AND APPLICATIONS
作者：PARK, Y;KIM, Y;CHANG, S
出处：CHEM REV 117 (13): 9247-9301 JUL 12 2017
地址：KOREA ADV INST SCI & TECHNOL, DEPT CHEM, DAEJEON 34141, SOUTH KOREA;INST FOR BASIC SCI KOREA, CTR CATALYT HYDROCARBON FUNCTIONALIZAT, DAEJEON 34141, SOUTH KOREA
摘要：Catalytic transformation of ubiquitous C-H bonds into valuable C-N bonds offers an efficient synthetic approach to construct N-functionalized molecules. Over the last few decades, transition metal catalysis has been repeatedly proven to be a powerful tool for the direct conversion of cheap hydrocarbons to synthetically versatile amino-containing compounds. This Review comprehensively highlights recent advances in intra- and intermolecular C-H amination reactions utilizing late transition metal based catalysts. Initial discovery, mechanistic study, and additional applications were

categorized on the basis of the mechanistic scaffolds and types of reactions. Reactivity and selectivity of novel systems are discussed in three sections, with each being defined by a proposed working mode.

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12.被引频次：306

题目：COLLOIDALLY PREPARED LA-DOPED BASNO3 ELECTRODES FOR EFFICIENT, PHOTOSTABLE PEROVSKITE SOLAR CELLS

作者：SHIN, SS;YEOM, EJ;YANG, WS;HUR, S;KIM, MG;IM, J;SEO, J;NOH, JH;SEOK, SI

出处：SCIENCE 356 (6334): 167-171 APR 14 2017

地址：KOREA RES INST CHEM TECHNOL, DIV ADV MAT, 141 GAJEONG RO, DAEJEON 34114, SOUTH KOREA;MIT, 77 MASSACHUSETTS AVE, CAMBRIDGE, MA 02139 USA;ULSAN NATL INST SCI & TECHNOL, SCH ENERGY & CHEM ENGN, PEROVTRON RES CTR, 50 UNIST GIL, ULSAN 44919, SOUTH KOREA;SEOUL NATL UNIV, DEPT MAT SCI & ENGN, SEOUL 151744, SOUTH KOREA;POHANG ACCELERATOR LAB, BEAMLINE RES DIV, POHANG 790784, SOUTH KOREA;KOREA UNIV, SCH CIVIL ENVIRONM & ARCHITECTURAL ENGN, SEOUL 136713, SOUTH KOREA

摘要：Perovskite solar cells (PSCs) exceeding a power conversion efficiency (PCE) of 20% have mainly been demonstrated by using mesoporous titanium dioxide (mp-TiO2) as an electron-transporting layer. However, TiO2 can reduce the stability of PSCs under illumination (including ultraviolet light). Lanthanum (La)-doped BaSnO3 (LBSO) perovskite would be an ideal replacement given its electron mobility and electronic structure, but LBSO cannot be synthesized as well-dispersible fine particles or crystallized below 500 degrees C. We report a superoxide colloidal solution route for preparing a LBSO electrode under very mild conditions (below 300 degrees C). The PSCs fabricated with LBSO and methylammonium lead iodide (MAPbI(3)) show a steady-state power conversion efficiency of 21.2%, versus 19.7% for a mp-TiO2 device. The LBSO-based PSCs could retain 93% of their initial performance after 1000 hours of full-Sun illumination.

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13.被引频次：289

题目：EARTH-ABUNDANT CATALYSTS FOR ELECTROCHEMICAL AND PHOTOELECTROCHEMICAL WATER SPLITTING

作者：ROGER, I;SHIPMAN, MA;SYMES, MD

出处：NAT REV CHEM 1 (1): - JAN 2017

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摘要：Sunlight is by far the most plentiful renewable energy resource, providing Earth with enough power to meet all of humanity's needs several hundred times over. However, it is both diffuse and intermittent, which presents problems regarding how best to harvest this energy and store it for times when the sun is not shining. Devices that use sunlight to split water into hydrogen and oxygen could be one solution to these problems, because hydrogen is an excellent fuel. However, if such devices are to become widely adopted, they must be cheap to produce and operate. Therefore, the development of electrocatalysts for water splitting that comprise only inexpensive, earth-abundant elements is critical. In this Review, we investigate progress towards such electrocatalysts, with

special emphasis on how they might be incorporated into photoelectrocatalytic water-splitting systems and the challenges that remain in developing these devices.
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14.被引频次：274
题目：FUSED NONACYCLIC ELECTRON ACCEPTORS FOR EFFICIENT POLYMER SOLAR CELLS
作者：DAI, SX;ZHAO, FW;ZHANG, QQ;LAU, TK;LI, TF;LIU, K;LING, QD;WANG, CR;LU, XH;YOU, W;ZHAN, XW
出处：J AM CHEM SOC 139 (3): 1336-1343 JAN 25 2017
地址：PEKING UNIV, DEPT MAT SCI & ENGN, KEY LAB POLYMER CHEM & PHYS, COLL ENGN,MINIST EDUC, BEIJING 100871, PEOPLES R CHINA;FUJIAN NORMAL UNIV, COLL MAT SCI & ENGN, FUJIAN KEY LAB POLYMER MAT, FUZHOU 350007, PEOPLES R CHINA;CHINESE ACAD SCI, INST CHEM, BEIJING 100190, PEOPLES R CHINA;UNIV NORTH CAROLINA CHAPEL HILL, DEPT CHEM, CHAPEL HILL, NC 27599 USA;CHINESE UNIV HONG KONG, DEPT PHYS, HONG KONG, HONG KONG, PEOPLES R CHINA
摘要：We design and synthesize four fused-ring electron acceptors based on-6,6,12,12-tetrakis(4-hexylphenyl)-indacenobis(dithieno[3,2-b-2',3'-d]thiophene) as the electron-rich unit and 1,1-dicyanomethylene-3-indanones with 0-2 fluorine substituents as the electron-deficient units. These four molecules exhibit broad (550-850 nm) and strong absorption with high extinction coefficients of (2.1-2.5) x 10(5) M-1 cm(-1). Fluorine substitution downshifts the LUMO energy level, red-shifts the absorption spectrum, and enhances electron mobility. The polymer solar cells based on the fluorinated electron acceptors exhibit power conversion efficiencies as high as 11.5%, much higher than that of their nonfluorinated counterpart (7.7%). We investigate the effects of the fluorine atom number and position on electronic properties, charge transport, film morphology, and photovoltaic properties.
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15.被引频次：267
题目：THE RAPID EVOLUTION OF HIGHLY EFFICIENT PEROVSKITE SOLAR CELLS
作者：CORREA-BAENA, JP;ABATE, A;SALIBA, M;TRESS, W;JACOBSSON, TJ;GRATZEL, M;HAGFELDT, A
出处：ENERGY ENVIRON SCI 10 (3): 710-727 MAR 1 2017
地址：ECOLE POLYTECH FED LAUSANNE, INST CHEM SCI & ENGN, LAB PHOTOMOL SCI, CH-1015 LAUSANNE, SWITZERLAND;ADOLPHE MERKLE INST, CHEMIN VERDIERS 4, CH-1700 FRIBOURG, SWITZERLAND;ECOLE POLYTECH FED LAUSANNE, INST CHEM SCI & ENGN, LAB PHOTON & INTERFACES, CH-1015 LAUSANNE, SWITZERLAND;UNIV CAMBRIDGE, DEPT CHEM, CHRISTIAN DOPPLER LAB SUSTAINABLE SYNGAS CHEM, CAMBRIDGE, ENGLAND;MIT, 77 MASSACHUSETTS AVE, CAMBRIDGE, MA 02139 USA
摘要：Perovskite solar cells (PSCs) have attracted much attention because of their rapid rise to 22% efficiencies. Here, we review the rapid evolution of PSCs as they enter a new phase that could revolutionize the photovoltaic industry. In particular, we describe the properties that make perovskites so remarkable, and the current understanding of the PSC device physics, including the operation of state-of-the-art solar cells with efficiencies above 20%. The extraordinary progress of

long-term stability is discussed and we provide an outlook on what the future of PSCs might soon bring the photovoltaic community. Some challenges remain in terms of reducing non-radiative recombination and increasing conductivity of the different device layers, and these will be discussed in depth in this review.
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16.被引频次：247
题目：TOWARD SAFE LITHIUM METAL ANODE IN RECHARGEABLE BATTERIES: A REVIEW
作者：CHENG, XB;ZHANG, R;ZHAO, CZ;ZHANG, Q
出处：CHEM REV 117 (15): 10403-10473 AUG 9 2017
地址：TSINGHUA UNIV, BEIJING KEY LAB GREEN CHEM REACT ENGN & TECHNOL, DEPT CHEM ENGN, BEIJING 100084, PEOPLES R CHINA
摘要：The lithium metal battery is strongly considered to be one of the most promising candidates for high-energy-density energy storage devices in our modern and technology-based society. However, uncontrollable lithium dendrite growth induces poor cycling efficiency and severe safety concerns, dragging lithium metal batteries out of practical applications. This review presents a comprehensive overview of the lithium metal anode and its dendritic lithium growth. First, the working principles and technical challenges of a lithium metal anode are underscored. Specific attention is paid to the mechanistic understandings and quantitative models for solid electrolyte interphase (SEI) formation, lithium dendrite nucleation, and growth. On the basis of previous theoretical understanding and analysis, recently proposed strategies to suppress dendrite growth of lithium metal anode and some other metal anodes are reviewed. A section dedicated to the potential of full-cell lithium metal batteries for practical applications is included. A general conclusion and a perspective on the current limitations and recommended future research directions of lithium metal batteries are presented. The review concludes with an attempt at summarizing the theoretical and experimental achievements in lithium metal anodes and endeavors to realize the practical applications of lithium metal batteries.
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17.被引频次：230
题目：RECENT ADVANCES IN ORGANIC THERMALLY ACTIVATED DELAYED FLUORESCENCE MATERIALS
作者：YANG, ZY;MAO, Z;XIE, ZL;ZHANG, Y;LIU, SW;ZHAO, J;XU, JR;CHI, ZG;ALDRED, MP
出处：CHEM SOC REV 46 (3): 915-1016 FEB 7 2017
地址：SUN YAT SEN UNIV, SCH CHEM,PCFM LAB, GUANGDONG ENGN TECHNOL RES CTR HIGHPERFORMANCE OR, STATE KEY LAB OPTOELECT MAT & TECHNOL,GD HPPC LAB, GUANGZHOU 510275, GUANGDONG, PEOPLES R CHINA;UNIV DURHAM, DEPT CHEM, DURHAM DH1 3LE, ENGLAND
摘要：Organic materials that exhibit thermally activated delayed fluorescence (TADF) are an attractive class of functional materials that have witnessed a booming development in recent years. Since Adachi et al. reported high-performance TADF-OLED devices in 2012, there have been many reports regarding the design and synthesis of new TADF luminogens, which have various molecular structures and are used for different applications. In this review, we summarize and discuss the latest progress concerning this rapidly developing research field, in which the majority of the reported

TADF systems are discussed, along with their derived structure-property relationships, TADF mechanisms and applications. We hope that such a review provides a clear outlook of these novel functional materials for a broad range of scientists within different disciplinary areas and attracts more researchers to devote themselves to this interesting research field.

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18.被引频次：224

题目：MOLECULAR MAGNETIC HYSTERESIS AT 60 KELVIN IN DYSPROSOCENIUM

作者：GOODWIN, CAP;ORTU, F;RETA, D;CHILTON, NF;MILLS, DP

出处：NATURE 548 (7668): 439-442 AUG 24 2017

地址：UNIV MANCHESTER, SCH CHEM, OXFORD RD, MANCHESTER M13 9PL, LANCS, ENGLAND

摘要：Lanthanides have been investigated extensively for potential applications in quantum information processing and high-density data storage at the molecular and atomic scale. Experimental achievements include reading and manipulating single nuclear spins(1,2), exploiting atomic clock transitions for robust qubits(3) and, most recently, magnetic data storage in single atoms(4,5). Single-molecule magnets exhibit magnetic hysteresis of molecular origin(6)-a magnetic memory effect and a prerequisite of data storage-and so far lanthanide examples have exhibited this phenomenon at the highest temperatures. However, in the nearly 25 years since the discovery of single-molecule magnets(7), hysteresis temperatures have increased from 4 kelvin to only about 14 kelvin(8-10) using a consistent magnetic field sweep rate of about 20 oersted per second, although higher temperatures have been achieved by using very fast sweep rates(11,12) (for example, 30 kelvin with 200 oersted per second)(12). Here we report a hexa-tert-butyldysprosocenium complex-[Dy(Cp-ttt)(2)][B(C6F5)(4)], with Cp-ttt = {(C5H2Bu3)-Bu-t-1,2,4} and Bu-t = C(CH3)(3)-which exhibits magnetic hysteresis at temperatures of up to 60 kelvin at a sweep rate of 22 oersted per second. We observe a clear change in the relaxation dynamics at this temperature, which persists in magnetically diluted samples, suggesting that the origin of the hysteresis is the localized metal-ligand vibrational modes that are unique to dysprosocenium. Ab initio calculations of spin dynamics demonstrate that magnetic relaxation at high temperatures is due to local molecular vibrations. These results indicate that, with judicious molecular design, magnetic data storage in single molecules at temperatures above liquid nitrogen should be possible.

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19.被引频次：223

题目：ELECTROCHEMICAL ADVANCED OXIDATION PROCESSES: A REVIEW ON THEIR APPLICATION TO SYNTHETIC AND REAL WASTEWATERS

作者：MOREIRA, FC;BOAVENTURA, RAR;BRILLAS, E;VILAR, VJP

出处：APPL CATAL B-ENVIRON 202: 217-261 MAR 2017

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摘要：Over the last decades, research efforts have been made at developing more effective technologies for the remediation of waters containing persistent organic pollutants. Among the

various technologies, the so-called electrochemical advanced oxidation processes (EAOPs) have caused increasing interest. These technologies are based on the electrochemical generation of strong oxidants such as hydroxyl radicals ((OH)-O-center dot). Here, we present an exhaustive review on the treatment of various synthetic and real wastewaters by five key EAOPs, i.e., anodic oxidation (AO), anodic oxidation with electrogenerated H2O2 (AO-H2O2), electro-Fenton (EF), photoelectro-Fenton (PEF) and solar photoelectro-Fenton (SPEF), alone and in combination with other methods like biological treatment, electrocoagulation, coagulation and membrane filtration processes. Fundamentals of each EAOP are also given. (C) 2016 Elsevier B.V. All rights reserved.
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20.被引频次：211
题目：METAL-ORGANIC FRAMEWORKS MEET METAL NANOPARTICLES: SYNERGISTIC EFFECT FOR ENHANCED CATALYSIS
作者：YANG, QH;XU, Q;JIANG, HL
出处：CHEM SOC REV 46 (15): 4774-4808 AUG 7 2017
地址：UNIV SCI & TECHNOL CHINA, HEFEI NATL LAB PHYS SCI MICROSCALE, CAS KEY LAB SOFT MATTER CHEM,DEPT CHEM, COLLABORAT INNOVAT CTR SUZHOU NANO SCI & TECHNOL, HEFEI 230026, ANHUI, PEOPLES R CHINA;NATL INST ADV IND SCI & TECHNOL, RES INST ELECTROCHEM ENERGY, 1-8-31 MIDORIGAOKA, IKEDA, OSAKA 5638577, JAPAN;KYOTO UNIV, CHEM ENERGY MAT OPEN INNOVAT LAB CHEM OIL, AIST, SAKYO KU, KYOTO 6068501, JAPAN
摘要：Metal-organic frameworks (MOFs), established as a relatively new class of crystalline porous materials with high surface area, structural diversity, and tailorability, attract extensive interest and exhibit a variety of applications, especially in catalysis. Their permanent porosity enables their inherent superiority in confining guest species, particularly small metal nanoparticles (MNPs), for improved catalytic performance and/or the expansion of reaction scope. This is a rapidly developing interdisciplinary research field. In this review, we provide an overview of significant progress in the development of MNP/MOF composites, including various preparation strategies and characterization methods as well as catalytic applications. Special emphasis is placed on synergistic effects between the two components that result in an enhanced performance in heterogeneous catalysis. Finally, the prospects of MNP/MOF composites in catalysis and remaining issues in this field have been indicated.
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21.被引频次：211
题目：A DYSPROSIUM METALLOCENE SINGLE-MOLECULE MAGNET FUNCTIONING AT THE AXIAL LIMIT
作者：GUO, FS;DAY, BM;CHEN, YC;TONG, ML;MANSIKKAMAKI, A;LAYFIELD, RA
出处：ANGEW CHEM INT ED 56 (38): 11445-11449 SEP 11 2017
地址：UNIV MANCHESTER, SCH CHEM, OXFORD RD, MANCHESTER M13 9PL, LANCS, ENGLAND;SUN YAT SEN UNIV, KEY LAB BIOINORGAN & SYNTHET CHEM, MINIST EDUC, SCH CHEM, GUANGZHOU 510275, GUANGDONG, PEOPLES R CHINA;UNIV JYVASKYLA, DEPT CHEM, NANOSCI CTR, POB 35, JYVASKYLA 40014, FINLAND
摘要：The Abstraction of a chloride ligand from the dysprosium metallocene [(Cp-ttt)(2)DyCl] (1(Dy)

Cp-ttt = 1,2,4-tri(tert-butyl)cyclopentadienide) by the triethylsilylium cation produces the first base-free rare-earth metallocenium cation [(Cp-ttt)(2)Dy](+) (2(Dy)) as a salt of the non-coordinating [B-(C6F5)(4)](-) anion. Magnetic measurements reveal that [2(Dy)][B-(C6F5)(4)] is an SMM with a record anisotropy barrier up to 1277 cm(-1) (1837 K) in zero field and a record magnetic blocking temperature of 60 K, including hysteresis with coercivity. The exceptional magnetic axiality of 2(Dy) is further highlighted by computational studies, which reveal this system to be the first lanthanide SMM in which all low-lying Kramers doublets correspond to a well-defined M-J value, with no significant mixing even in the higher doublets.

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22.被引频次：208

题目：METAL-ORGANIC FRAMEWORKS FOR HETEROGENEOUS BASIC CATALYSIS

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出处：CHEM REV 117 (12): 8129-8176 JUN 28 2017

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摘要：Great attention has been given to metal organic frameworks (MOFs)derived solid bases because of their attractive structure and catalytic performance in :various organic reactions. The extraordinary skeleton structure of MOFs provides many possibilities for incorporation of diverse basic functionalities, which is unachievable for conventional solid bases. The past decade has witnessed remarkable advances in this vibrant research area; however, MOFs for heterogeneous basic catalysis have never been reviewed until now. Therefore, a review summarizing MOFs-derived base catalysts is highly expected. In this review, we present an overview of the recent progress in MOFs-derived solid bases covering preparation, characterization, and catalytic applications. In the preparation section, the solid bases are divided into two categories, namely, MOFs with intrinsic basicity and MOFs with modified basicity. The basicity can originate from either metal sites or organic ligands. Different approaches used for generation of basic sites are included, and each approach is described with representative examples. The fundamental principles for the design and fabrication of MOFs with basic functionalities are featured. In the characterization section, experimental techniques and theoretical calculations employed for characterization of basic MOFs are summarized. Some representive experimental techniques, such as temperature-programmed desorption of CO2 (CO2-TPD) and infrared (IR) spectra of different probing molecules, are covered. Following preparation and characterization, the catalytic applications of MOFs-derived solid bases are dealt with. These solid bases have potential to catalyze some well-known "base-catalyzed reactions" like Knoevenagel condensation, aldol condensation, and Michael addition. Meanwhile, in contrast to conventional solid bases, MOFs show some different catalytic properties due to their special structural and surface properties. Remarkably, characteristic features of MOFs-derived solid bases are described by comparing with conventional inorganic counterparts, keeping in mind the current opportunities and challenges in this field.

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23.被引频次：202
题目：THE ATOM, THE MOLECULE, AND THE COVALENT ORGANIC FRAMEWORK
作者：DIERCKS, CS;YAGHI, OM
出处：SCIENCE 355 (6328): - MAR 3 2017
地址：UNIV CALIF BERKELEY, DEPT CHEM, BERKELEY, CA 94720 USA;LAWRENCE BERKELEY NATL LAB, DIV MAT SCI, BERKELEY, CA 94720 USA;KAVLI ENERGY NANOSCI INST, BERKELEY, CA 94720 USA;BERKELEY GLOBAL SCI INST, BERKELEY, CA 94720 USA;KING ABDULAZIZ CITY SCI & TECHNOL, RIYADH 11442, SAUDI ARABIA
摘要：Just over a century ago, Lewis published his seminal work on what became known as the covalent bond, which has since occupied a central role in the theory of making organic molecules. With the advent of covalent organic frameworks (COFs), the chemistry of the covalent bond was extended to two-and three-dimensional frameworks. Here, organic molecules are linked by covalent bonds to yield crystalline, porous COFs from light elements (boron, carbon, nitrogen, oxygen, and silicon) that are characterized by high architectural and chemical robustness. This discovery paved the way for carrying out chemistry on frameworks without losing their porosity or crystallinity, and in turn achieving designed properties in materials. The recent union of the covalent and the mechanical bond in the COF provides the opportunity for making woven structures that incorporate flexibility and dynamics into frameworks.
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24.被引频次：198
题目：OXIDATIVE C-H/C-H COUPLING REACTIONS BETWEEN TWO (HETERO)ARENES
作者：YANG, YD;LAN, JB;YOU, JS
出处：CHEM REV 117 (13): 8787-8863 JUL 12 2017
地址：SICHUAN UNIV, COLL CHEM, MINIST EDUC, KEY LAB GREEN CHEM & TECHNOL, 29 WANGJIANG RD, CHENGDU 610064, PEOPLES R CHINA
摘要：Transition metal-mediated C-H bond activation and functionalization represent one of the most straightforward and powerful tools in modern organic synthetic chemistry. Bi(hetero)aryls are privileged pi-conjugated structural cores in biologically active molecules, organic functional materials, ligands, and organic synthetic intermediates. The oxidative C-H/C-H coupling reactions between two (hetero)arenes through 2-fold C-H activation offer a valuable opportunity for rapid assembly of diverse bi(hetero)aryls and further exploitation of their applications in pharmaceutical and material sciences. This review provides a comprehensive overview of the fundamentals and applications of transition metal-mediated/catalyzed oxidative C-H/C-H coupling reactions between two (hetero)arenes. The substrate scope, limitation, reaction mechanism, regioselectivity, and chemoselectivity, as well as related control strategies of these reactions are discussed. Additionally, the applications of these established methods in the synthesis of natural products and exploitation of new organic functional materials are exemplified. In the last section, a short introduction on oxidant- or Lewis acid-mediated oxidative Ar-H/Ar-H coupling reactions is presented, considering that it is a very powerful method for the construction of biaryl units and polycylic arenes.
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25.被引频次：197
题目：SELF-TEMPLATING SYNTHESIS OF HOLLOW CO3O4 MICROTUBE ARRAYS FOR HIGHLY EFFICIENT WATER ELECTROLYSIS
作者：ZHU, YP;MA, TY;JARONIEC, M;QIAO, SZ
出处：ANGEW CHEM INT ED 56 (5): 1324-1328 JAN 24 2017
地址：UNIV ADELAIDE, SCH CHEM ENGN, ADELAIDE, SA 5005, AUSTRALIA;KENT STATE UNIV, DEPT CHEM & BIOCHEM, KENT, OH 44240 USA
摘要：In spite of recent advances in the synthesis of hollow micro/nanostructures, the fabrication of three-dimensional electrodes on the basis of these structures remains a major challenge. Herein, we develop an electrochemical sacrificial-template strategy to fabricate hollow Co3O4 microtube arrays with hierarchical porosity. The resultant unique structures and integrated electrode configurations impart enhanced mass transfer and electron mobility, ensuring high activity and stability in catalyzing oxygen and hydrogen evolution reactions. Impressively, the apparent performance can rival that of state-of-the-art noble-metal and transition-metal electrocatalysts. Furthermore, this bifunctional electrode can be used for highly efficient overall water splitting, even competing with the integrated performance of Pt/C and IrO2/C.
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ESI HIGHLY CITED PAPERS

(Chemistry)

（来源：http://esi.incites.thomsonreuters.com）

1.被引频次：59292
题目：A SHORT HISTORY OF SHELX
作者：SHELDRICK, GM
出处：ACTA CRYSTALLOGR A 64: 112-122 PART 1 JAN 2008
地址：UNIV GOTTINGEN, DEPT STRUCT CHEM, D-37077 GOTTINGEN, GERMANY
摘要：An account is given of the development of the SHELX system of computer programs from SHELX-76 to the present day. In addition to identifying useful innovations that have come into general use through their implementation in SHELX, a critical analysis is presented of the less-successful features, missed opportunities and desirable improvements for future releases of the software. An attempt is made to understand how a program originally designed for photographic intensity data, punched cards and computers over 10000 times slower than an average modern personal computer has managed to survive for so long. SHELXL is the most widely used program for small-molecule refinement and SHELXS and SHELXD are often employed for structure solution

despite the availability of objectively superior programs. SHELXL also finds a niche for the refinement of macromolecules against high-resolution or twinned data; SHELXPRO acts as an interface for macromolecular applications. SHELXC, SHELXD and SHELXE are proving useful for the experimental phasing of macromolecules, especially because they are fast and robust and so are often employed in pipelines for high-throughput phasing. This paper could serve as a general literature citation when one or more of the open-source SHELX programs (and the Bruker AXS version SHELXTL) are employed in the course of a crystal-structure determination.

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2.被引频次：11313

题目：THE M06 SUITE OF DENSITY FUNCTIONALS FOR MAIN GROUP THERMOCHEMISTRY, THERMOCHEMICAL KINETICS, NONCOVALENT INTERACTIONS, EXCITED STATES, AND TRANSITION ELEMENTS: TWO NEW FUNCTIONALS AND SYSTEMATIC TESTING OF FOUR M06-CLASS FUNCTIONALS AND 12 OTHER FUNCTIONALS

作者：ZHAO, Y;TRUHLAR, DG

出处：THEOR CHEM ACC 120 (1-3): 215-241 MAY 2008

地址：UNIV MINNESOTA, DEPT CHEM, MINNEAPOLIS, MN 55455 USA;UNIV MINNESOTA, DEPT CHEM, INST SUPERCOMP, MINNEAPOLIS, MN 55455 USA

摘要：We present two new hybrid meta exchange-correlation functionals, called M06 and M06-2X. The M06 functional is parametrized including both transition metals and nonmetals, whereas the M06-2X functional is a high-nonlocality functional with double the amount of nonlocal exchange (2X), and it is parametrized only for nonmetals. The functionals, along with the previously published M06-L local functional and the M06-HF full-Hartree-Fock functionals, constitute the M06 suite of complementary functionals. We assess these four functionals by comparing their performance to that of 12 other functionals and Hartree-Fock theory for 403 energetic data in 29 diverse databases, including ten databases for thermochemistry, four databases for kinetics, eight databases for noncovalent interactions, three databases for transition metal bonding, one database for metal atom excitation energies, and three databases for molecular excitation energies. We also illustrate the performance of these 17 methods for three databases containing 40 bond lengths and for databases containing 38 vibrational frequencies and 15 vibrational zero point energies. We recommend the M06-2X functional for applications involving main-group thermochemistry, kinetics, noncovalent interactions, and electronic excitation energies to valence and Rydberg states. We recommend the M06 functional for application in organometallic and inorganometallic chemistry and for noncovalent interactions.

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3.被引频次：9264

题目：A CONSISTENT AND ACCURATE AB INITIO PARAMETRIZATION OF DENSITY FUNCTIONAL DISPERSION CORRECTION (DFT-D) FOR THE 94 ELEMENTS H-PU

作者：GRIMME, S;ANTONY, J;EHRLICH, S;KRIEG, H

出处：J CHEM PHYS 132 (15): - APR 21 2010

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摘要：The method of dispersion correction as an add-on to standard Kohn-Sham density functional theory (DFT-D) has been refined regarding higher accuracy, broader range of applicability, and less empiricism. The main new ingredients are atom-pairwise specific dispersion coefficients and cutoff radii that are both computed from first principles. The coefficients for new eighth-order dispersion terms are computed using established recursion relations. System (geometry) dependent information is used for the first time in a DFT-D type approach by employing the new concept of fractional coordination numbers (CN). They are used to interpolate between dispersion coefficients of atoms in different chemical environments. The method only requires adjustment of two global parameters for each density functional, is asymptotically exact for a gas of weakly interacting neutral atoms, and easily allows the computation of atomic forces. Three-body nonadditivity terms are considered. The method has been assessed on standard benchmark sets for inter- and intramolecular noncovalent interactions with a particular emphasis on a consistent description of light and heavy element systems. The mean absolute deviations for the S22 benchmark set of noncovalent interactions for 11 standard density functionals decrease by 15%-40% compared to the previous (already accurate) DFT-D version. Spectacular improvements are found for a tripeptide-folding model and all tested metallic systems. The rectification of the long-range behavior and the use of more accurate C-6 coefficients also lead to a much better description of large (infinite) systems as shown for graphene sheets and the adsorption of benzene on an Ag(111) surface. For graphene it is found that the inclusion of three-body terms substantially (by about 10%) weakens the interlayer binding. We propose the revised DFT-D method as a general tool for the computation of the dispersion energy in molecules and solids of any kind with DFT and related (low-cost) electronic structure methods for large systems.

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4.被引频次：8237

题目：GROMACS 4: ALGORITHMS FOR HIGHLY EFFICIENT, LOAD-BALANCED, AND SCALABLE MOLECULAR SIMULATION

作者：HESS, B;KUTZNER, C;VAN DER SPOEL, D;LINDAHL, E

出处：J CHEM THEORY COMPUT 4 (3): 435-447 MAR 2008

地址：MAX PLANCK INST POLYMER RES, D-55128 MAINZ, GERMANY;MAX PLANCK INST BIOPHYS CHEM, DEPT THEORET & COMPUTAT BIOPHYS, D-37077 GOTTINGEN, GERMANY;UPPSALA UNIV, DEPT CELL & MOL BIOL, SE-75124 UPPSALA, SWEDEN;STOCKHOLM UNIV, STOCKHOLM CTR BIOMEMBRANE RES, SE-10691 STOCKHOLM, SWEDEN

摘要：Molecular simulation is an extremely useful, but computationally very expensive tool for studies of chemical and biomolecular systems. Here, we present a new implementation of our molecular simulation toolkit GROMACS which now both achieves extremely high performance on single processors from algorithmic optimizations and hand-coded routines and simultaneously scales very well on parallel machines. The code encompasses a minimal-communication domain decomposition algorithm, full dynamic load balancing, a state-of-the-art parallel constraint solver, and efficient virtual site algorithms that allow removal of hydrogen atom degrees of freedom to enable integration time steps up to 5 fs; for atomistic simulations also in parallel. To improve the scaling properties of the common particle mesh Ewald electrostatics algorithms, we have in addition used a Multiple-Program, Multiple-Data approach, with separate node domains responsible for direct and reciprocal space interactions. Not only does this combination of algorithms enable extremely

long simulations of large systems but also it provides that simulation performance on quite modest numbers of standard cluster nodes.
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5.被引频次：8054
题目：BUILDING BETTER BATTERIES
作者：ARMAND, M;TARASCON, JM
出处：NATURE 451 (7179): 652-657 FEB 7 2008
地址：UNIV PICARDIE, LRCS, CNRS, UMR 6007, AMIENS, FRANCE
摘要：
电子邮件：jean-marie.tarascon@sc.u-picardie.fr

6.被引频次：6737
题目：CRYSTAL STRUCTURE REFINEMENT WITH SHELXL
作者：SHELDRICK, GM
出处：ACTA CRYSTALLOGR C 71: 3-8 PART 1 JAN 2015
地址：UNIV GOTTINGEN, DEPT STRUCT CHEM, D-37077 GOTTINGEN, GERMANY
摘要：The improvements in the crystal structure refinement program SHELXL have been closely coupled with the development and increasing importance of the CIF (Crystallographic Information Framework) format for validating and archiving crystal structures. An important simplification is that now only one file in CIF format (for convenience, referred to simply as 'a CIF') containing embedded reflection data and SHELXL instructions is needed for a complete structure archive; the program SHREDCIF can be used to extract the .hkl and .ins files required for further refinement with SHELXL. Recent developments in SHELXL facilitate refinement against neutron diffraction data, the treatment of H atoms, the determination of absolute structure, the input of partial structure factors and the refinement of twinned and disordered structures. SHELXL is available free to academics for the Windows, Linux and Mac OS X operating systems, and is particularly suitable for multiple-core processors.
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7.被引频次：5601
题目：THE CHEMISTRY OF GRAPHENE OXIDE
作者：DREYER, DR;PARK, S;BIELAWSKI, CW;RUOFF, RS
出处：CHEM SOC REV 39 (1): 228-240 2010
地址：UNIV TEXAS AUSTIN, DEPT CHEM & BIOCHEM, AUSTIN, TX 78712 USA;UNIV TEXAS AUSTIN, DEPT MECH ENGN, TEXAS MAT INST, AUSTIN, TX 78712 USA
摘要：The chemistry of graphene oxide is discussed in this critical review. Particular emphasis is directed toward the synthesis of graphene oxide, as well as its structure. Graphene oxide as a substrate for a variety of chemical transformations, including its reduction to graphene-like materials, is also discussed. This review will be of value to synthetic chemists interested in this emerging field of materials science, as well as those investigating applications of graphene who would find a more thorough treatment of the chemistry of graphene oxide useful in understanding the scope and limitations of current approaches which utilize this material (91 references).
电子邮件：bielawski@cm.utexas.edu; r.ruoff@mail.utexas.edu

8.被引频次：5472

题目：ORGANOMETAL HALIDE PEROVSKITES AS VISIBLE-LIGHT SENSITIZERS FOR PHOTOVOLTAIC CELLS

作者：KOJIMA, A;TESHIMA, K;SHIRAI, Y;MIYASAKA, T

出处：J AM CHEM SOC 131 (17): 6050-+ MAY 6 2009

地址：UNIV TOKYO, GRAD SCH ARTS & SCI, MEGURO KU, TOKYO 1538902, JAPAN;TOIN UNIV YOKOHAMA, GRAD SCH ENGN, AOBA KU, KANAGAWA 2258502, JAPAN;PECCELL TECHNOL INC, AOBA KU, KANAGAWA 2258502, JAPAN;TOKYO POLYTECH UNIV, GRAD SCH ENGN, KANAGAWA 2430297, JAPAN

摘要：Two organolead halide perovskite nanocrystals, CH3NH3PbBr3 and CH(3)NH(3)Pbl(3), were found to efficiently sensitize TiO2 for visible-light conversion in photoetectrochemical cells. When self-assembled on mesoporous TiO2 films, the nanocrystattine perovskites exhibit strong band-gap absorptions as semiconductors. The CH(3)NH(3)Pbl(3)-based photocell with spectral sensitivity of up to 800 nm yielded a solar energy conversion efficiency of 3.8%. The CH3NH3PbBr3-based cell showed a high photovoltage of 0.96 V with an external quantum conversion efficiency of 65%.

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9.被引频次：5316

题目：IRON-BASED LAYERED SUPERCONDUCTOR LA[O1-XFX]FEAS (X=0.05-0.12) WITH T-C=26 K

作者：KAMIHARA, Y;WATANABE, T;HIRANO, M;HOSONO, H

出处：J AM CHEM SOC 130 (11): 3296-+ MAR 19 2008

地址：TOKYO INST TECHNOL, FRONTIER RES CTR, JST, ERATO SORST,MIDORI KU, YOKOHAMA, KANAGAWA 2268503, JAPAN;TOKYO INST TECHNOL, MAT & STRUCT LAB, MIDORI KU, YOKOHAMA, KANAGAWA 2268503, JAPAN

摘要：We report that a layered iron-based compound LaOFeAs undergoes superconducting transition under doping with P ions at the O2- site. The transition temperature (T-c) exhibits a trapezoid shape dependence on the F- content, with the highest T. of similar to 26 K at -11 atom %.

电子邮件：hosono@msl.titech.ac.ip

10.被引频次：5245

题目：DYE-SENSITIZED SOLAR CELLS

作者：HAGFELDT, A;BOSCHLOO, G;SUN, LC;KLOO, L;PETTERSSON, H

出处：CHEM REV 110 (11): 6595-6663 NOV 2010

地址：UPPSALA UNIV, DEPT PHYS & ANALYT CHEM, SE-75105 UPPSALA, SWEDEN;KTH ROYAL INST TECHNOL, DEPT CHEM, SE-10044 STOCKHOLM, SWEDEN;DALIAN UNIV TECHNOL, STATE KEY LAB FINE CHEM, DUT KTH JOINT EDUC & RES CTR MOL DEVICES, DALIAN 116012, PEOPLES R CHINA;SWEREA IVF AB, SE-43122 MOLNDAL, SWEDEN

摘要：

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11.被引频次：5056
题目：SOFTWARE NEWS AND UPDATE AUTODOCK VINA: IMPROVING THE SPEED AND ACCURACY OF DOCKING WITH A NEW SCORING FUNCTION, EFFICIENT OPTIMIZATION, AND MULTITHREADING
作者：TROTT, O;OLSON, AJ
出处：J COMPUT CHEM 31 (2): 455-461 JAN 30 2010
地址：SCRIPPS RES INST, DEPT MOL BIOL, LA JOLLA, CA 92037 USA
摘要：AutoDock Vina, a new program for molecular docking and virtual screening, is presented. AutoDock Vina achieves an approximately two orders of magnitude speed-up compared with the molecular docking software previously developed in our lab (AutoDock 4), while also significantly improving the accuracy of the binding mode predictions, judging by our tests on the training set used in AutoDock 4 development. Further speed-up is achieved from parallelism, by using multithreading on multicore machines. AutoDock Vina automatically calculates the grid maps and clusters the results in a way transparent to the user. (C) 2009 Wiley Periodicals, Inc. J Comput Chem 31: 455-461, 2010
电子邮件：olson@scripps.edu

12.被引频次：4908
题目：HETEROGENEOUS PHOTOCATALYST MATERIALS FOR WATER SPLITTING
作者：KUDO, A;MISEKI, Y
出处：CHEM SOC REV 38 (1): 253-278 2009
地址：TOKYO UNIV SCI, FAC SCI, SHINJUKU KU, TOKYO 1621861, JAPAN
摘要：This critical review shows the basis of photocatalytic water splitting and experimental points, and surveys heterogeneous photocatalyst materials for water splitting into H(2) and O(2), and H(2) or O(2) evolution from an aqueous solution containing a sacrificial reagent. Many oxides consisting of metal cations with d(0) and d(10) configurations, metal (oxy) sulfide and metal (oxy) nitride photocatalysts have been reported, especially during the latest decade. The fruitful photocatalyst library gives important information on factors affecting photocatalytic performances and design of new materials. Photocatalytic water splitting and H(2) evolution using abundant compounds as electron donors are expected to contribute to construction of a clean and simple system for solar hydrogen production, and a solution of global energy and environmental issues in the future (361 references).
电子邮件：kudo@rs.kagu.tus.ac.jp

13.被引频次：4732
题目：AUTODOCK4 AND AUTODOCKTOOLS4: AUTOMATED DOCKING WITH SELECTIVE RECEPTOR FLEXIBILITY
作者：MORRIS, GM;HUEY, R;LINDSTROM, W;SANNER, MF;BELEW, RK;GOODSELL, DS;OLSON, AJ
出处：J COMPUT CHEM 30 (16): 2785-2791 DEC 30 2009
地址：SCRIPPS RES INST, DEPT MOL BIOL, LA JOLLA, CA 92037 USA;UNIV CALIF SAN DIEGO, DEPT COGNIT SCI, LA JOLLA, CA 92093 USA
摘要：We describe the testing and release of AutoDock4 and the accompanying graphical user interface AutoDockTools. AutoDock4 incorporates limited flexibility in the receptor. Several tests are

reported here, including a redocking experiment with 188 diverse ligand-protein complexes and a cross-docking experiment using flexible side-chains in 87 HIV protease complexes. We also report its utility in analysis of covalently bound ligands, using both a grid-based clocking method and a modification of the flexible sidechain technique. (C) 2009 Wiley Periodicals, Inc. J Comput Chem 30: 2785-2791, 2009
电子邮件：olson@scripps.edu

14.被引频次：4507
题目：SEQUENTIAL DEPOSITION AS A ROUTE TO HIGH-PERFORMANCE PEROVSKITE-SENSITIZED SOLAR CELLS
作者：BURSCHKA, J;PELLET, N;MOON, SJ;HUMPHRY-BAKER, R;GAO, P;NAZEERUDDIN, MK;GRATZEL, M
出处：NATURE 499 (7458): 316-+ JUL 18 2013
地址：SWISS FED INST TECHNOL, DEPT CHEM & CHEM ENGN, LAB PHOTON & INTERFACES, CH-1015 LAUSANNE, SWITZERLAND;MAX PLANCK INST SOLID STATE RES, D-70569 STUTTGART, GERMANY
摘要：Following pioneering work(1), solution-processable organic-inorganic hybrid perovskites-such as CH3NH3PbX3 (X = Cl, Br, I)-have attracted attention as light-harvesting materials for mesoscopic solar cells(2-15). So far, the perovskite pigment has been deposited in a single step onto mesoporous metal oxide films using a mixture of PbX2 and CH3NH3X in a common solvent. However, the uncontrolled precipitation of the perovskite produces large morphological variations, resulting in a wide spread of photovoltaic performance in the resulting devices, which hampers the prospects for practical applications. Here we describe a sequential deposition method for the formation of the perovskite pigment within the porous metal oxide film. PbI2 is first introduced from solution into a nanoporous titanium dioxide film and subsequently transformed into the perovskite by exposing it to a solution of CH3NH3I. We find that the conversion occurs within the nanoporous host as soon as the two components come into contact, permitting much better control over the perovskite morphology than is possible with the previously employed route. Using this technique for the fabrication of solid-state mesoscopic solar cells greatly increases the reproducibility of their performance and allows us to achieve a power conversion efficiency of approximately 15 per cent (measured under standard AM1.5G test conditions on solar zenith angle, solar light intensity and cell temperature). This two-step method should provide new opportunities for the fabrication of solution-processed photovoltaic cells with unprecedented power conversion efficiencies and high stability equal to or even greater than those of today's best thin-film photovoltaic devices.
电子邮件：michael.graetzel@epfl.ch

15.被引频次：4454
题目：EFFICIENT HYBRID SOLAR CELLS BASED ON MESO-SUPERSTRUCTURED ORGANOMETAL HALIDE PEROVSKITES
作者：LEE, MM;TEUSCHER, J;MIYASAKA, T;MURAKAMI, TN;SNAITH, HJ
出处：SCIENCE 338 (6107): 643-647 NOV 2 2012
地址：UNIV OXFORD, DEPT PHYS, CLARENDON LAB, OXFORD OX1 3PU, ENGLAND;TOIN UNIV YOKOHAMA, GRAD SCH ENGN, AOBA KU, YOKOHAMA, KANAGAWA 2258503, JAPAN;NATL INST ADV IND SCI & TECHNOL, RES CTR

PHOTOVOLTA TECHNOL, TSUKUBA, IBARAKI 3058565, JAPAN

摘要：The energy costs associated with separating tightly bound excitons (photoinduced electron-hole pairs) and extracting free charges from highly disordered low-mobility networks represent fundamental losses for many low-cost photovoltaic technologies. We report a low-cost, solution-processable solar cell, based on a highly crystalline perovskite absorber with intense visible to near-infrared absorptivity, that has a power conversion efficiency of 10.9% in a single-junction device under simulated full sunlight. This "meso-superstructured solar cell" exhibits exceptionally few fundamental energy losses; it can generate open-circuit photovoltages of more than 1.1 volts, despite the relatively narrow absorber band gap of 1.55 electron volts. The functionality arises from the use of mesoporous alumina as an inert scaffold that structures the absorber and forces electrons to reside in and be transported through the perovskite.

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16.被引频次：4445

题目：METAL-ORGANIC FRAMEWORK MATERIALS AS CATALYSTS

作者：LEE, J;FARHA, OK;ROBERTS, J;SCHEIDT, KA;NGUYEN, ST;HUPP, JT

出处：CHEM SOC REV 38 (5): 1450-1459 2009

地址：NORTHWESTERN UNIV, DEPT CHEM, EVANSTON, IL 60208 USA

摘要：A critical review of the emerging. field of MOF-based catalysis is presented. Discussed are examples of: (a) opportunistic catalysis with metal nodes, (b) designed catalysis with framework nodes, (c) catalysis by homogeneous catalysts incorporated as framework struts, (d) catalysis by MOF-encapsulated molecular species, (e) catalysis by metal-free organic struts or cavity modifiers, and (f) catalysis by MOF-encapsulated clusters (66 references).

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17.被引频次：4341

题目：SELECTIVE GAS ADSORPTION AND SEPARATION IN METAL-ORGANIC FRAMEWORKS

作者：LI, JR;KUPPLER, RJ;ZHOU, HC

出处：CHEM SOC REV 38 (5): 1477-1504 2009

地址：TEXAS A&M UNIV, DEPT CHEM, COLLEGE STN, TX 77842 USA

摘要：Adsorptive separation is very important in industry. Generally, the process uses porous solid materials such as zeolites, activated carbons, or silica gels as adsorbents. With an ever increasing need for a more efficient, energy-saving, and environmentally benign procedure for gas separation, adsorbents with tailored structures and tunable surface properties must be found. Metal-organic frameworks (MOFs), constructed by metal-containing nodes connected by organic bridges, are such a new type of porous materials. They are promising candidates as adsorbents for gas separations due to their large surface areas, adjustable pore sizes and controllable properties, as well as acceptable thermal stability. This critical review starts with a brief introduction to gas separation and purification based on selective adsorption, followed by a review of gas selective adsorption in rigid and flexible MOFs. Based on possible mechanisms, selective adsorptions observed in MOFs are classified, and primary relationships between adsorption properties and framework features are analyzed. As a specific example of tailor-made MOFs, mesh-adjustable molecular sieves are emphasized and the underlying working mechanism elucidated. In addition to the experimental aspect, theoretical investigations from adsorption equilibrium to diffusion dynamics via molecular simulations are also briefly reviewed. Furthermore, gas separations in MOFs, including the molecular sieving effect, kinetic separation, the quantum sieving effect for H-2/D-2 separation, and MOF-based membranes are also summarized (227 references).

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18.被引频次：4261

题目：SOLAR WATER SPLITTING CELLS

作者：WALTER, MG;WARREN, EL;MCKONE, JR;BOETTCHER, SW;MI, QX;SANTORI, EA;LEWIS, NS

出处：CHEM REV 110 (11): 6446-6473 NOV 2010

地址：CALTECH, DIV CHEM & CHEM ENGN, NOYES LAB 210, PASADENA, CA 91125 USA

摘要：

电子邮件：nslewis@caltech.edu

19.被引频次：4192

题目：PORPHYRIN-SENSITIZED SOLAR CELLS WITH COBALT (II/III)-BASED REDOX ELECTROLYTE EXCEED 12 PERCENT EFFICIENCY

作者：YELLA, A;LEE, HW;TSAO, HN;YI, CY;CHANDIRAN, AK;NAZEERUDDIN, MK;DIAU, EWG;YEH, CY;ZAKEERUDDIN, SM;GRATZEL, M

出处：SCIENCE 334 (6056): 629-634 NOV 4 2011

地址：NATL CHIAO TUNG UNIV, DEPT APPL CHEM, HSINCHU 300, TAIWAN;NATL CHIAO TUNG UNIV, INST MOL SCI, HSINCHU 300, TAIWAN;ECOLE POLYTECH FED LAUSANNE, INST CHEM SCI & ENGN, LAB PHOTON & INTERFACES, CH-1015 LAUSANNE, SWITZERLAND;NATL CHUNG HSING UNIV, DEPT CHEM, TAICHUNG 402, TAIWAN;NATL CHUNG HSING UNIV, CTR NANOSCI & NANOTECHNOL, TAICHUNG 402, TAIWAN

摘要：The iodide/triiodide redox shuttle has limited the efficiencies accessible in dye-sensitized solar cells. Here, we report mesoscopic solar cells that incorporate a Co((II/III))tris(bipyridyl)-based redox electrolyte in conjunction with a custom synthesized donor-pi-bridge-acceptor zinc porphyrin dye as sensitizer (designated YD2-o-C8). The specific molecular design of YD2-o-C8 greatly retards the rate of interfacial back electron transfer from the conduction band of the nanocrystalline titanium dioxide film to the oxidized cobalt mediator, which enables attainment of strikingly high photovoltages approaching 1 volt. Because the YD2-o-C8 porphyrin harvests sunlight across the visible spectrum, large photocurrents are generated. Cosensitization of YD2-o-C8 with another organic dye further enhances the performance of the device, leading to a measured power conversion efficiency of 12.3% under simulated air mass 1.5 global sunlight.

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20.被引频次：4126

题目：VESTA 3 FOR THREE-DIMENSIONAL VISUALIZATION OF CRYSTAL, VOLUMETRIC AND MORPHOLOGY DATA

作者：MOMMA, K;IZUMI, F

出处：J APPL CRYST 44: 1272-1276 PART 6 DEC 2011

地址：NATL INST MAT SCI, QUANTUM BEAM UNIT, TSUKUBA, IBARAKI 3050044, JAPAN

摘要：VESTA is a three-dimensional visualization system for crystallographic studies and electronic state calculations. It has been upgraded to the latest version, VESTA 3, implementing new features including drawing the external morphology of crystals; superimposing multiple structural models, volumetric data and crystal faces; calculation of electron and nuclear densities from structure parameters; calculation of Patterson functions from structure parameters or volumetric data; integration of electron and nuclear densities by Voronoi tessellation; visualization of isosurfaces with multiple levels; determination of the best plane for selected atoms; an extended bond-search algorithm to enable more sophisticated searches in complex molecules and cage-like structures; undo and redo in graphical user interface operations; and significant performance improvements in rendering isosurfaces and calculating slices.

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21.被引频次：4077

题目：UNIVERSAL SOLVATION MODEL BASED ON SOLUTE ELECTRON DENSITY AND ON A CONTINUUM MODEL OF THE SOLVENT DEFINED BY THE BULK DIELECTRIC CONSTANT AND ATOMIC SURFACE TENSIONS

作者：MARENICH, AV;CRAMER, CJ;TRUHLAR, DG

出处：J PHYS CHEM B 113 (18): 6378-6396 MAY 7 2009

地址：UNIV MINNESOTA, DEPT CHEM, MINNEAPOLIS, MN 55455 USA;UNIV MINNESOTA, INST SUPERCOMP, MINNEAPOLIS, MN 55455 USA

摘要：We present a new continuum solvation model based on the quantum mechanical charge density of a solute molecule interacting with a continuum description of the solvent. The model is called SMD, where the "D". stands for "density" to denote that the full solute electron density is used without defining partial atomic charges. "Continuum" denotes that the solvent is not represented explicitly but rather as a dielectric medium with surface tension at the solute-solvent boundary. SMD is a universal solvation model, where "universal" denotes its applicability to any charged or uncharged solute in any solvent or liquid medium for which a few key descriptors are known (in particular, dielectric constant, refractive index, bulk surface tension, and acidity and basicity parameters). The model separates the observable solvation free energy into two main components. The first component is the bulk electrostatic contribution arising from a self-consistent reaction field treatment that involves the solution of the nonhomogeneous Poisson equation for electrostatics in terms of the integral-equation-formalism polarizable continuum model (IEF-PCM). The cavities for the bulk electrostatic calculation are defined by superpositions of nuclear-centered spheres. The second component is called the cavity-dispersion-solvent- structure term and is the contribution arising from short-range interactions between the solute and solvent molecules in the first solvation shell. This contribution is a sum of terms that are proportional (with geometry-dependent proportionality constants called atomic surface tensions) to the solvent-accessible surface areas of the individual atoms of the solute. The SMD model has been parametrized with a training set of 2821 solvation data including 112 aqueous ionic solvation free energies, 220 solvation free energies for 166 ions in acetonitrile, methanol, and dimethyl sulfoxide, 2346 solvation free energies for 318 neutral solutes in 91 solvents (90 nonaqueous organic solvents and water), and 143 transfer free energies for 93 neutral solutes between water and 15 organic solvents. The elements present in the solutes are H, C, N, O, F, Si, P, S, Cl, and Br. The SMD model employs a single set of parameters

(intrinsic atomic Coulomb radii and atomic surface tension coefficients) optimized over six electronic structure methods: M05-2X/MIDI!6D, M05-2X/6-31G*, M05-2X/6-31+G**, M05-2X/cc-pVTZ, B3LYP/6-31G*, and HF/6-31G*. Although the SMD model has been parametrized using the IEF-PCM protocol for bulk electrostatics, it may also be employed with other algorithms for solving the nonhomogeneous Poisson equation for continuum solvation calculations in which the solute is represented by its electron density in real space. This includes, for example, the conductor-like screening algorithm. With the 6-31G* basis set, the SMD model achieves mean unsigned errors of 0.6-1.0 kcal/mol in the solvation free energies of tested neutrals and mean unsigned errors of 4 kcal/mol on average for ions with either Gaussian03 or GAMESS.
电子邮件：cramer@umn.edu; truhlar@umn.edu

22.被引频次：3915
题目：HYBRID POROUS SOLIDS: PAST, PRESENT, FUTURE
作者：FEREY, G
出处：CHEM SOC REV 37 (1): 191-214 2008
地址：UNIV VERSAILLES ST QUENTIN YVELINES, INST LAVOISIER, CNRS, UMR 8180, F-78035 VERSAILLES, FRANCE
摘要：This critical review will be of interest to the experts in porous solids (including catalysis), but also solid state chemists and physicists. It presents the state-of-the-art on hybrid porous solids, their advantages, their new routes of synthesis, the structural concepts useful for their 'design', aiming at reaching very large pores. Their dynamic properties and the possibility of predicting their structure are described. The large tunability of the pore size leads to unprecedented properties and applications. They concern adsorption of species, storage and delivery and the physical properties of the dense phases.
电子邮件：ferey@chimie.uvsq.fr

23.被引频次：3903
题目：LONG-RANGE CORRECTED HYBRID DENSITY FUNCTIONALS WITH DAMPED ATOM-ATOM DISPERSION CORRECTIONS
作者：CHAI, JD;HEAD-GORDON, M
出处：PHYS CHEM CHEM PHYS 10 (44): 6615-6620 2008
地址：UNIV CALIF BERKELEY, DEPT CHEM, BERKELEY, CA 94720 USA;LAWRENCE BERKELEY LAB, BERKELEY, CA 94720 USA
摘要：We report re-optimization of a recently proposed long-range corrected (LC) hybrid density functional [J.-D. Chai and M. Head-Gordon, J. Chem. Phys., 2008, 128, 084106] to include empirical atom-atom dispersion corrections. The resulting functional, omega B97X-D yields satisfactory accuracy for thermochemistry, kinetics, and non-covalent interactions. Tests show that for non-covalent systems, omega B97X-D shows slight improvement over other empirical dispersion-corrected density functionals, while for covalent systems and kinetics it performs noticeably better. Relative to our previous functionals, such as omega B97X, the new functional is significantly superior for non-bonded interactions, and very similar in performance for bonded interactions.
电子邮件：mhg@cchem.berkeley.edu

24.被引频次：3850
题目：ELECTRICAL ENERGY STORAGE FOR THE GRID: A BATTERY OF CHOICES
作者：DUNN, B;KAMATH, H;TARASCON, JM
出处：SCIENCE 334 (6058): 928-935 NOV 18 2011
地址：UNIV CALIF LOS ANGELES, DEPT MAT SCI & ENGN, LOS ANGELES, CA 90095 USA;UNIV CALIF LOS ANGELES, CALIF NANOSYST INST, LOS ANGELES, CA 90095 USA;ELECT POWER RES INST, PALO ALTO, CA 94304 USA;UNIV PICARDIE JULES VERNE, LAB REACT CHIM SOLIDES, F-80039 AMIENS, FRANCE;COLL FRANCE, F-75231 PARIS, FRANCE
摘要：The increasing interest in energy storage for the grid can be attributed to multiple factors, including the capital costs of managing peak demands, the investments needed for grid reliability, and the integration of renewable energy sources. Although existing energy storage is dominated by pumped hydroelectric, there is the recognition that battery systems can offer a number of high-value opportunities, provided that lower costs can be obtained. The battery systems reviewed here include sodium-sulfur batteries that are commercially available for grid applications, redox-flow batteries that offer low cost, and lithium-ion batteries whose development for commercial electronics and electric vehicles is being applied to grid storage.
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25.被引频次：3832
题目：DENSITY FUNCTIONALS WITH BROAD APPLICABILITY IN CHEMISTRY
作者：ZHAO, Y;TRUHLAR, DG
出处：ACCOUNT CHEM RES 41 (2): 157-167 FEB 2008
地址：UNIV MINNESOTA, DEPT CHEM, MINNEAPOLIS, MN 55455 USA;UNIV MINNESOTA, INST SUPERCOMP, MINNEAPOLIS, MN 55455 USA
摘要：
电子邮件：truhlar@umn.edu

AIAA、AAS、IAF 最新会议

AIAA

（AIAA 来源：http://www.aiaa.org/）

1.会议名称： 66th Annual Reliability & Maintainability Symposium (RAMS)
会议时间：27 - 30 January 2020
会议地点：Palm Springs, California
会议简介：The 66th Annual Reliability & Maintainability Symposium (RAMS®) will be held at the

Marriott Renaissance in Palm Springs, CA during the week of January 27-30, 2020. The theme for RAMS® 2020 is “R&M in a Model-based System Engineering Environment”.

The evolution of autonomous systems, artificial intelligence, new levels of complexity in human-machine interface design, and maintainability decisions have intensified the critical role of RAMS® disciplines. Integrating design elements from concept to final design that replicates actual working environments is the challenge industry faces today. The RAMS® 2020 theme offers a broad umbrella of opportunities for presenting papers and tutorials that address theory and application of RAMS® disciplines in the design, development and support process; and how these disciplines can be applied to new technologies through lessons learned, analyses, modeling, and simulation. Equally important is the discussion on the classical approaches, spanning all technologies, and disciplines focusing on optimizing performance.

With this in mind, we invite you to share the theoretical or practical findings of your research, engineering case studies, success stories, lessons learned, R&M based analyses and simulations, or R&M discoveries at RAMS® 2020 Palm Springs. Tell us how you are designing, optimizing, and supporting systems (both hardware and software) through the execution of RAMS® disciplines.

链接：http://www.rams.org/

2.**会议名称：**2020 IEEE Aerospace Conference
会议时间：7 - 14 March 2020
会议地点：Big Sky, Montana
会议简介：The international IEEE Aerospace Conference, with AIAA and PHM Society as technical cosponsors, is organized to promote interdisciplinary understanding of aerospace systems, their underlying science and technology, and their applications to government and commercial endeavors.
链接：https://www.aiaa.org/2020-IEEE-Aerospace-Conference/

3.**会议名称：**27th Saint Petersburg International Conference on Integrated Navigation System
会议时间：25 - 27 May 2020
会议地点：Saint Petersburg, Russia
会议简介：The 27th Saint Petersburg International Conference on Integrated Navigation Systems will be held by the State Research Center of the Russian Federation - Concern Central Scientific and Research Institute Elektropribor, JSC, on 25-27 May 2020.
链接：https://www.aiaa.org/27th-St-Petersburg-ICINS/

AAS

（AAS 来源：http://astronautical.org/）

1.**会议名称：** AAS/AIAA Astrodynamics Specialist Conference
会议时间：August 10-15, 2019
会议地点：Portland, Maine
会议简介：The 2018 AAS/AIAA Astrodynamics Specialist Conference hosted by the American Astronautical Society (AAS) and co-hosted by the American Institute of Aeronautics and Astronautics (AIAA) will be held August 19-23, 2018 at the Cliff Lodge in Snowbird, UT. The

conference is organized by the AAS Space Flight Mechanics Committee and the AIAA Astrodynamics Technical Committee.
链接：http://www.space-flight.org/docs/2018_summer/2018_summer.html

IAF

（IAF 来源：http://www.iafastro.org/）

1.**会议名称：**AEC2020 Conference
会议时间：25 - 28 February 2020
会议地点：Bordeaux, France
会议简介：To pave the way for a single European aerospace conference, 3AF and CEAS have decided to join forces to launch the very first edition of the Aerospace Europe Conference (AEC2020).
Aerospace Europe Conference 2020, will feature 3AF 3rd Greener Aviation, CEAS 7th Air & Space Conference and the 8th edition of Aircraft Noise and Emissions Reduction Symposium (ANERS).
This conference will be offering scientists and engineers from industry, government, and academia an exceptional opportunity to exchange knowledge and results of current studies and to discuss directions for future research in the fields of aeronautics and space. Individually, each of the three conferences has proven to be very successful. In joining the three we expect to be even more attractive, offering additional transversal topics and synergies between aeronautics and space towards a greener and cleaner environment.
By welcoming worldwide contributions, this new conference will give attendees a unique overview of the global research efforts aimed at reducing the environmental impact of aviation and space activities.
链接：https://aerospace-europe2020.eu/

2. **会议名称：**SpaceOps 2020 Conference
会议时间：18 - 22 May 2020
会议地点：Cape Town, South Africa
会议简介：As the chairman of the local organisation committee and representative of the South African National Space Agency (SANSA), I look forward to welcoming you to Cape Town, South Africa from 18 – 22 May 2020 for SpaceOps 2020.
SpaceOps 2020, hosted by SANSA, will provide the opportunity for you to share experiences, challenges, and innovative solutions with colleagues from around the world. This conference aims to bring together the global space operations community to address state-of-the-art operations principles, methods and tools. Held biennially since 1990, the conference attracts technologists, scientists, and managers from space agencies, industry, and academia, and fosters managerial and technical interchange on all aspects of space mission operations, including robotic and human spaceflight, Earth orbit and deep space missions, lunar and planetary missions, and orbital and surface operations.
SpaceOps 2020 will be held for the first time on the African continent, in the multicultural melting pot with a rich history, Cape Town, South Africa. South Africa is rapidly taking its place amongst the scientific destinations of choice with the science and technology innovations & research it undertakes

on a global scale. Our country, South Africa, also offers the discerning tourist an exciting mix of tourist and entertainment possibilities. Visitors will find Cape Town a vibrant, trendy, sophisticated, well connected and stunningly attractive modern city to visit. South Africa's top 6 tourist attractions are within an hour from the City Centre with SpaceOps 2020 right in the centre of it all.

链接：http://www.spaceops2020.org/

ACM 最新会议

来源：http://www.acm.org/

1. **会议名称：**ASONAM 2019

会议时间： 27-30 August, 2019

会议地点：Vancouver, Canada

会议简介：For more than a century, social networks have been studied in a variety of disciplines including sociology, anthropology, psychology, and economics. The Internet, the social Web, and other large-scale, socio-technological infrastructures have triggered a growing interest and significant methodological advancements in social network analysis and mining. Method development in graph theory, statistics, data mining and machine learning, and statistical mechanics is inspired by new research problems and, in turn, opens up further possibilities for application. These spiraling trends have led to a rising prominence of social network analysis and mining methods and tools in academia, politics, security, and business.

The international conference series on Advances in Social Network Analysis and Mining (ASONAM 2019) provides an interdisciplinary venue that brings together researchers and practitioners from a broad variety of fields to promote collaborations and exchange of ideas and practices. ASONAM 2019 is intended to address important aspects with a specific focus on emerging trends and industry needs. The conference solicits empirical, experimental, methodological, and theoretical research reporting original and unpublished results on social network analysis and mining along with applications.

Full papers will be reviewed and assessed by the program committee and a "Best Paper Award" ceremony will be organized at the banquet.

链接：http://asonam.cpsc.ucalgary.ca/2019/

2.**会议名称：**ICICM 2019

会议时间：August 23-26, 2019

会议地点：Prague, Czech Republic

会议简介：Welcome to the official website of The 9th International Conference on Information Communication and Management (ICICM 2019). ICICM is an annual conference which aims to present the latest research and results of scientists (professors, doctoral students, and post-doc scientists) related to Information Communication and Management topics. This conference provides opportunities for delegates from different areas to exchange new ideas, applications and experiences face to face, to establish business or research relations, and to find global partners for future collaboration. We hope that the conference results in significant contributions to the knowledge base in these scientific fields. The conference has been held in Singapore, Hong Kong, Paris (France), Geneva (Switzerland), Paris (France), Hatfield (England), Moscow (Russia), and Edinburgh (Scotland) in the past 8 years.

ICICM 2019 will be held on August 23-26, 2019 in Prague, Czech Republic features invited keynote speakers as well as peer-reviewed paper presentations.The conference is completely open (one needs to register first), you will not have to be an author or a discussant to attend.

链接：http://www.icicm.org/

3.**会议名称：**ESEC/FSE 2019
会议时间：26-30 AUGUST 2019
会议地点：TALLINN, ESTONIA
会议简介：The 27th ACM Joint European Software Engineering Conference and Symposium on the Foundations of Software Engineering (ESEC/FSE) is an internationally renowned forum for researchers, practitioners, and educators to present and discuss the most recent innovations, trends, experiences, and challenges in the field of software engineering.

ESEC/FSE conference brings together experts from academia and industry to exchange the latest research results and trends, as well as their practical application in all areas of software engineering.

We invite high-quality submissions describing original and unpublished results of theoretical, empirical, conceptual, and experimental software engineering research. We also welcome multi-disciplinary work at the interface between software engineering and other related topics, such as, but not restricted to, artificial intelligence, human computer interaction, programming languages, and systems engineering. The flyer with the call for papers for all tracks can be downloaded here.

ESEC/FSE’19 will be held in the conference centre of Sokos Hotel Viru in the modern city of Tallinn. Tallinn has a long history as an important trade centre in the Northern Baltic Sea region. Today, it is the vibrant capital of Estonia, the European leader in the development and promotion of an information society.

链接：https://esec-fse19.ut.ee/

4.**会议名称：**ACM BCB 2019
会议时间：September 7-10, 2019
会议地点：Niagara Falls, New York
会议简介：The 10th ACM Conference on Bioinformatics, Computational Biology, and Health Informatics (ACM BCB) is the flagship conference of the ACM SIGBio. ACM-BCB 2019 is the conference's tenth year, building upon the success of the first eight meetings in Boston, Niagara Falls, Chicago, Orlando, Washington DC, Newport Beach, Atlanta, and Seattle. ACM-BCB 2019 will be held in Niagara Falls, New York, September 7-10, 2019.

The conference is a premier dissemination forum for interdisciplinary research linking computer science, mathematics, statistics, biology, bioinformatics, biomedical informatics, and health informatics. The past few decades have seen tremendous growth in the scale and complexity of biological and medical data including recent mainstream recognition of big data challenges. This conference serves to showcase leading-edge research on new technologies and techniques around gathering, processing, analyzing, and modeling of data and information for a variety of scientific, clinical, and healthcare applications, from bench to bedside.

This year, we are pleased to announce that the Workshop on Algorithms in Bioinformatics (WABI) will be co-located with ACM-BCB.

链接：http://acm-bcb.org/2019/index.php

5.**会议名称：**13th ACM Conference on Recommender Systems

会议时间：16th-20th September 2019

会议地点：Copenhagen, Denmark

会议简介：The ACM Recommender Systems conference (RecSys) is the premier international forum for the presentation of new research results, systems and techniques in the broad field of recommender systems. Recommendation is a particular form of information filtering, that exploits past behaviors and user similarities to generate a list of information items that is personally tailored to an end-user's preferences. As RecSys brings together the main international research groups working on recommender systems, along with many of the world's leading e-commerce companies, it has become the most important annual conference for the presentation and discussion of recommender systems research. RecSys 2019, the thirteenth conference in this series, will be held in Copenhagen, Denmark. It will bring together researchers and practitioners from academia and industry to present their latest results and identify new trends and challenges in providing recommendation components in a range of innovative application contexts. In addition to the main technical track, RecSys 2019 program will feature keynote and invited talks, tutorials covering state-of-the-art in this domain, a workshop program, an industrial track and a doctoral symposium.

Published papers will go through a rigorous full peer review process. The conference proceedings, which will be available both on a USB drive and via the ACM Digital Library, are expected to be widely read and cited.

链接：http://recsys.acm.org/recsys19/

6.**会议名称：**AUTOUI'19

会议时间：SEPTEMBER 22-25, 2019

会议地点：UTRECHT,NETHERLANDS

会议简介：AutomotiveUI (or short: AutoUI) is the International ACM SIGCHI Conference on Automotive User Interfaces and Interactive Vehicular Applications. It is the premier forum for UI research in the automotive domain. The conference annually brings together over 200 researchers and practitioners interested in both the technical and the human aspects of in-vehicle user interfaces and applications, to provide a forum for the exchange of technical information concerning research (and practice) and educational activities for motor vehicle user interface development. We have multiple meeting categories in which researchers, practitioners, and other interested parties can take part in our conference and community. We welcome you to engage with us in this exciting field!

链接：https://www.auto-ui.org/19/

7.**会议名称：**MEMSYS 2019

会议时间：Sept. 30 – Oct 3

会议地点：Washington, DC

会议简介：Memory-device manufacturing, memory-architecture design, and the use of memory technologies by application software all profoundly impact today's and tomorrow's computing systems, in terms of their performance, function, reliability, predictability, power dissipation, and cost. Existing memory technologies are seen as limiting in terms of power, capacity, and bandwidth. Emerging memory technologies offer the potential to overcome both technology- and design-related limitations to answer the requirements of many different applications. Our goal is to bring together researchers, practitioners, and others interested in this exciting and rapidly evolving field, to update each other on the latest state of the art, to exchange ideas, and to discuss future challenges.

链接：https://memsys.io/

8.**会议名称：**HAI 2019

会议时间：6-10th October 2019

会议地点：Kyoto, Japan

会议简介：HAI 2019 is the 7th annual International Conference on Human-Agent Interaction. It is a venue with an interdisciplinary nature to discuss and disseminate state-of-the-art research on topics that relate to human interactions with a range of agent systems, including physical robots, virtual agents, socially interactive agents, and artificially intelligent agents.

The theme for HAI 2019 is“Human-Agent Interaction, the Heart of Artificial Intelligence.”

Due to the rapid progress of deep learning, AI has reached a human or superhuman level in image recognition and games such as Go and is approaching the level of human in speech recognition, translation, automatic driving, and many other applications. It can be said that Human-Agent Interaction (HAI) has now become the most exciting target area of AI.

While all submissions related to HAI are welcome as usual, you are especially encouraged to submit papers in line with the theme for HAI 2019, "Human-Agent Interaction, the Heart of Artificial Intelligence." We are looking forward to sharing the latest research results of HAI that contribute to elucidate the mechanism of intelligence, implementation reports of groundbreaking HAI utilizing cutting-edge AI technology, and advanced research results of the boundary region between HAI and AI such as interactive machine learning and human-AI partnerships.

Full papers, posters, late-breaking results, and tutorial/workshop overviews will be archived in the ACM Digital Library.

链接：http://hai-conference.net/hai2019/

9.**会议名称：**ACM Inaugural Symposium on Computer Science and Law

会议时间：October 28 and 29, 2019

会议地点：New York City

会议简介：The main goals of the inaugural ACM Symposium on Computer Science and Law are to stimulate interest in computer science and law, broadly defined, and to articulate a research agenda, an educational agenda, and specific recommendations about how ACM and other interested institutions can support work in this emerging field. The Symposium will take place at the New York Law School in the Tribeca neighborhood of New York City on October 28 and 29, 2019.

链接：https://computersciencelaw.org/

10.**会议名称：**IEEE/ACM International Symposium on Microarchitecture®

会议时间：October 12-16, 2019

会议地点：Columbus, Ohio

会议简介：The IEEE/ACM International Symposium on Microarchitecture® is the premier forum for presenting, discussing, and debating innovative microarchitecture ideas and techniques for advanced computing and communication systems. This symposium brings together researchers in fields related to microarchitecture, compilers, chips, and systems for technical exchange on traditional microarchitecture topics and emerging research areas. The MICRO community has enjoyed a close interaction between academic researchers and industrial designers.

链接：https://www.microarch.org/

IQPC 最新国防会议(Defence)

IQPC 来源：http://www.iqpc.com/

1. **会议名称：**Military Radar
会议时间：28 - 30 August, 2019
会议地点：London
会议简介：The emergence of new hypersonic systems, next generation capabilities and low, slow, small drone systems has placed a renewed emphasis on the ability of military operators to identify, monitor and track potential threats.

Military Radar 2019 has been designed to support the operator against the new threat by exploring and assessing the next phase of radar capability. Focussing on new developments in 3D phased array radar, cognitive and passive radar viability in theatre, and the implications of autonomy in AESA radar and Airborne Surveillance Systems

Ahead of the significant system updates over the next 5 years, the military radar conference will demonstrate the full extent of the programme, exploring the latest in academic research, technical capacity and industry capability to inform the programme, and challenge industry to present new creative approaches to the future of radar.

Join a panel of experts at the 17th annual Military Radar summit, as they establish a critical path for applying advanced radar technology to address new challenges. Take part in the only summit committed not just to realising the latest research, but to understanding how this research is being applied by the world's leading defence agencies.

链接：https://militaryradar.iqpc.co.uk/?utm_medium=portal&mac=IQPCCORP

2.**会议名称：**Offshore Patrol Vessels International
会议时间：24 - 26 September, 2019
会议地点：Spain
会议简介：The International Offshore Patrol Vessel conference will be hosted by the Spanish Navy in 2019.With the EU NAVFOR Headquarters moving from the UK to Rota Naval Base in Cadiz Spain, the conference will provide a timely opportunity to engage with senior officers involved in this mission as well as see the expertise of the conference's industrial partner, Cluster Maritimo

Naval Cádiz. In advancing these discussions, the 2019 edition will acknowledge an increasingly complex maritime security environment; an environment which demands an updated assessment of the role of the OPV platform itself. Indeed, the need to understand the potential roles across the spectrum of conflict is growing in such a complex environment – should for instance the OPV concept include adaptability and readiness to contribute to a high-intensity conflict scenario? Engaging in debate about where this type of platform sits within the broader constabulary and battle fleet is critical, if such concepts are to sustain their relevance and deliver robust capabilities for the future.

Offshore Patrol Vessels 2018 was the most international year in the event's history. Representatives from over 25 nations attended, including Canada, Ghana, the USA, Malaysia, Oman, Colombia, Brazil, Ecuador and Portugal, this is your only opportunity to address the challenges facing the global OPV community, as they seek to define a future role for this critical maritime security platform.

Join us in September 2019 as we work to maximise situational awareness, upgrade inherent baseline capability and deliver a continuous patrol function for the OPV.

链接：https://offshorepatrolvessels.iqpc.co.uk/?utm_medium=portal&mac=IQPCCORP

3.会议名称：Directed Energy Systems

会议时间：29 - 31 October, 2019

会议地点：London, UK

会议简介：The theme for DES 2018 is "Transitioning to The Warfighter". While technical and scientific elements will be covered the focus will be on the future of militarily useful DE and the next steps required for these systems to earn their way onto platforms and into operations.

We are undoubtedly at a time where Directed Energy Systems are moving on to platforms across the tri-service. Technological progress is helping to meet SWaP-C challenges and the spectrum of threats-faced now includes UAVs and smaller targets which require, and provide operational rationale, for lower powered systems. At the same time missile defence requires the future operationalisation of high-powered systems. The race is on to field systems now, get this technology into the hands of the Warfighter, gain feedback on how the systems can be used and take an iterative approach to refine and design future systems.

DES 2018 will contribute to the dialogue and expose capability planners, future operators and researchers to case-studies, developments in other nations, and help militaries share TTPS and Operational Concepts for this new capability. No more promises, DE is moving into operations!

链接：https://directedenergysystems.iqpc.co.uk/?utm_medium=portal&mac=IQPCCORP

4.会议名称：ISR and C2 Battle Management USA

会议时间：November 05 - 07, 2019

会议地点：Hilton Crystal City at Washington Reagan National Airport, Arlington, WA

会议简介：The ISR & C2 Battle Management U.S conference is an important strategic forum for the Five Eyes partners, welcoming over 150 senior decision-makers from across the Army, Air Force, Navy and DOD to discuss major procurement programs, reflect on operational challenges, and share strategic thinking on C2ISR.

The 5th annual event is themed around 'Shaping the Multi-Domain Imperative, from Concept to Capability'. As the U.S. and its Five Eyes partners transition towards the multi-domain paradigm, we are confronted with myriad technological, organisational and practical challenges in turning this

concept into a reality, in an era where acquisition must adapt and innovate at the speed of relevance. This year's event will be a unique joint dialogue on the multi-domain operational concept, the new Air Force ISR Flight Plan, and the other emerging ideas and technologies shaping strategic decision making in the C2ISR enterprise today.
链接：https://isrusa.iqpc.com/?utm_medium=portal&mac=IQPCCORP

5.**会议名称：**Future Indirect Fires Eastern Europe
会议时间：20 - 21 November, 2019
会议地点：Prague
会议简介：We are incredibly pleased to announce the Future Indirect Fires Eastern Europe conference taking place between 27-29 November 2018 in Prague, Czech Republic.

The rapidly changing operating environment has prompted many militaries to initiate vigorous modernisation programmes and continue investing resources into the training of personnel. The Czech Republic recently launched an ambitious procurement plan which includes digitisation of fires C2, and the acquisition of NATO standardised 155mm howitzers and 120mm mortar systems. Other European nations have also announced tenders to modernise existing assets, procure NATO compliant platforms, and attain interoperability in response to Russian aggression om the Eastern flank.

In light of the NATO Enhanced Forward Presence operation, it is evermore critical to support allied nation's fires initiatives and advance firepower by upgrading precision engagement, target acquisition, and long-range fire support capability. All this in an operating environment that requires careful signature management.

The Future Indirect Fires Eastern Europe Conference will provide a comprehensive account of indirect fires modernisation priorities, battlespace integration, mobility and mechanisation, reconnaissance & surveillance, target identification, smart munitions, electronic warfare, and information & cyberspace operations.
链接：https://indirectfires.iqpc.co.uk/?utm_medium=portal&mac=IQPCCORP

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