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最新学科研究热点与前沿

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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服务部承担。“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 最新会议，由 AIAA、AAS 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、内容编排等有好的意见和建议，欢迎与我们联系(电话：88492928)，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

2020 年 4 月

目 录

NatureLatest Research(Chemistry)

来源：https://www.nature.com/nchem/

1. **标题：**The synthesis, properties and potential applications of cyclic polymers
作者：Farihah M. Haque & Scott M. Grayson
摘要：Unlike their more common linear counterparts, cyclic polymers have a ring-like structure and a lack of chain ends. Because of their topology, cyclic polymers exhibit a unique set of properties when compared with linear or branched macromolecules. For example, cyclic homopolymers exhibit a reduced hydrodynamic volume and a slower degradation profile compared with their linear analogues. Cyclic block copolymers self-assemble into compact nanostructures, as illustrated by their reduced domain spacing when cast into thin films and their reduced micellar size in solution. Although methods for preparing well-defined cyclic polymers have only been available since 1980, the extensive utilization of the cyclic topology in nature highlights the vital role that a cyclic architecture can play in imparting valuable physical properties, such as increased chemical stability or propensity towards self-assembly. This Review describes the major developments in the synthesis of cyclic polymers and provides an overview of their fundamental physical properties. In this context, preliminary studies exploring potential applications will be critically assessed and the remaining challenges for the field delineated.
链接：https://www.nature.com/articles/s41557-020-0440-5

2. **标题：**Directional conformer exchange in dihydrofolate reductase revealed by single-molecule nanopore recordings
作者：Nicole Stéphanie Galenkamp, Annemie Biesemans & Giovanni Maglia
摘要：Conformational heterogeneity is emerging as a defining characteristic of enzyme function. However, understanding the role of protein conformations requires their thermodynamic and kinetic characterization at the single-molecule level, which remains extremely challenging. Here we report the ligand-induced conformational changes of dihydrofolate reductase (DHFR) by measuring the modulation of the nanopore currents. The long observation time of the electrical recordings enabled the detection of rare conformational transitions hidden in ensemble measurements. We show that DHFR exists in at least four ground-state configurations or conformers with different affinities for its ligands. Unliganded DHFR adopted low-affinity conformers, whereas the binding of substrates promoted the switch to the high-affinity conformer. Conversion between the conformers was accelerated by molecules that stabilized the transition state of DHFR, which suggests that the reaction lowers the energy barrier for conformer exchange and thus facilitates product release. This mechanism might be a general feature in enzymatic reactions affected by product inhibition or when the release of products is the rate-limiting step.
链接：https://www.nature.com/articles/s41557-020-0437-0

3.**标题：**Rapid functionalization of multiple C–H bonds in unprotected alicyclic amines

作者：Weijie Chen, Anirudra Paul, Khalil A. Abboud & Daniel Seidel

摘要：The synthesis of valuable bioactive alicyclic amines containing variable substituents in multiple ring positions typically relies on multistep synthetic sequences that frequently require the introduction and subsequent removal of undesirable protecting groups. Although a vast number of studies have aimed to simplify access to such materials through the C–H bond functionalization of feedstock alicyclic amines, the simultaneous introduction of more than one substituent to unprotected amines has never been accomplished. Here we report an advance in C–H bond functionalization methodology that enables the introduction of up to three substituents in a single operation. Lithiated amines are first exposed to a ketone oxidant, generating transient imines that are subsequently converted to endocyclic 1-azaallyl anions, which can be processed further to furnish β-substituted, α,β-disubstituted, or α,β,α′-trisubstituted amines. This study highlights the unique utility of in situ-generated endocyclic 1-azaallyl anions, elusive intermediates in synthetic chemistry.

链接：https://www.nature.com/articles/s41557-020-0438-z

4.**标题：**Total synthesis of terpenes via palladium-catalysed cyclization strategy

作者：Barry M. Trost & Chang Min

摘要：Nature’s synthetic plans to construct molecules have been developed over millions of years of evolution and frequently prove to be among the most sophisticated. Mimicking nature’s route can be a direct and feasible way for synthetic organic chemists to construct complicated molecules. However, lacking nature’s ability to manipulate enzymes often prevents us from reproducing the same route. Modifying nature’s approaches can provide a simpler synthetic alternative to access complex structural target molecules. Here we report a strategy that simplifies the synthesis of terpenes by inverting the order of nature’s two-phase biosynthesis route. We first unite simple molecules into a polyfunctionalized linear polyenyne, with all the desired carbons and oxygens in the targeted places. This compound then undergoes polyenyne cycloisomerization, in the presence of all the functional groups, to give polyoxidized terpenes. The key reaction is a palladium-catalysed polyenyne cycloisomerization that not only tolerates the presence of all of the oxygen functionalities, but also is facilitated by them.

链接：https://www.nature.com/articles/s41557-020-0439-y

5.**标题：**Understanding metal synergy in heterodinuclear catalysts for the copolymerization of CO2 and epoxides

作者：Arron C. Deacy, Alexander F. R. Kilpatrick, Anna Regoutz & Charlotte K. Williams

摘要：Carbon dioxide and epoxide copolymerization is an industrially relevant means to valorize waste and improve sustainability in polymer manufacturing. Given the value of the polymer products—polycarbonates or polyether carbonates—it could provide an economic stimulus to capture and storage technologies. The process efficiency depends upon the catalyst, and previously Zn(II)Mg(II) heterodinuclear catalysts showed good performances at low carbon dioxide pressures, attributed to synergic interactions between the metals. Now, a Mg(II)Co(II) catalyst is reported that exhibits significantly better activity (turnover frequency > 12,000 h−1) and high selectivity (>99% CO2 utilization and polycarbonate selectivity) for carbon dioxide and cyclohexene oxide copolymerization. Detailed kinetic investigations show a second-order rate law, independent of CO2

pressure from 1–40 bar, to produce polyols. Kinetic data also reveal that synergy arises from differentiated roles for the metals in the mechanism: epoxide coordination occurs at Mg(II), with reduced transition state entropy, while the Co(II) centre accelerates carbonate attack by lowering the transition state enthalpy. This rare insight into intermetallic synergy rationalizes the outstanding catalytic performance and provides a new feature to exploit in other homogeneous catalyses.
链接：https://www.nature.com/articles/s41557-020-0450-3

6. **标题：**Multi-responsive hydrogel structures from patterned droplet networks
作者：Florence G. Downs, David J. Lunn, Michael J. Booth, Joshua B. Sauer, William J. Ramsay, R. George Klemperer, Craig J. Hawker & Hagan Bayley
摘要：Responsive hydrogels that undergo controlled shape changes in response to a range of stimuli are of interest for microscale soft robotic and biomedical devices. However, these applications require fabrication methods capable of preparing complex, heterogeneous materials. Here we report a new approach for making patterned, multi-material and multi-responsive hydrogels, on a micrometre to millimetre scale. Nanolitre aqueous pre-gel droplets were connected through lipid bilayers in predetermined architectures and photopolymerized to yield continuous hydrogel structures. By using this droplet network technology to pattern domains containing temperature-responsive or non-responsive hydrogels, structures that undergo reversible curling were produced. Through patterning of gold nanoparticle-containing domains into the hydrogels, light-activated shape change was achieved, while domains bearing magnetic particles allowed movement of the structures in a magnetic field. To highlight our technique, we generated a multi-responsive hydrogel that, at one temperature, could be moved through a constriction under a magnetic field and, at a second temperature, could grip and transport a cargo.
链接：https://www.nature.com/articles/s41557-020-0444-1

7.**标题：**Chemoselective oxidative generation of ortho-quinone methides and tandem transformations
作者：Muhammet Uyanik, Kohei Nishioka, Ryutaro Kondo & Kazuaki Ishihara
摘要：ortho-Quinone methides are useful transient synthetic intermediates in organic synthesis. These species are most often generated in situ by the acid- or base-mediated transformation of phenols that have been pre-functionalized at a benzylic position, or by biomimetic oxidation of the corresponding ortho-alkylphenols with metal oxidants or transition-metal complexes. Here we describe a method for the transition-metal-free oxidative generation of o-QMs from ortho-alkylarenols, using hypoiodite catalysis under nearly neutral conditions, which can then be applied in one-pot tandem reactions. This method for the chemoselective oxidative generation of ortho-quinone methides may prove superior to previous methods with respect to environmental issues and scope, and can be applied to various tandem reactions such as inter- or intramolecular [4 + 2] cycloaddition, oxa-6π-electrocyclization, conjugate addition and spiroepoxidation.
链接：https://www.nature.com/articles/s41557-020-0433-4

8.**标题：**Demystifying the asymmetry-amplifying, autocatalytic behaviour of the Soai reaction through structural, mechanistic and computational studies
作者：Soumitra V. Athavale, Adam Simon, Kendall N. Houk & Scott E. Denmark
摘要：The Soai reaction has profoundly impacted chemists' perspective of autocatalysis, chiral

symmetry breaking, absolute asymmetric synthesis and its role in the origin of biological homochirality. Here we describe the unprecedented observation of asymmetry-amplifying autocatalysis in the alkylation of 5-(trimethylsilylethynyl)pyridine-3-carbaldehyde using diisopropylzinc. Kinetic studies with a surrogate substrate and spectroscopic analysis of a series of zinc alkoxides that incorporate specific structural mutations reveal a 'pyridine-assisted cube escape'. The new tetrameric cluster functions as a catalyst that activates the substrate through a two-point binding mode and poises a coordinated diisopropylzinc moiety for alkyl group transfer. Transition-state models leading to both the homochiral and heterochiral products were validated by density functional theory calculations. Moreover, experimental and computational analysis of the heterochiral complex provides a definitive explanation for the nonlinear behaviour of this system. Our deconstruction of the Soai system reveals the structural logic for autocatalyst evolution, function and substrate compatibility—a central mechanistic aspect of this iconic transformation.

链接：https://www.nature.com/articles/s41557-020-0421-8

9. **标题：** Delayed fluorescence from a zirconium(IV) photosensitizer with ligand-to-metal charge-transfer excited states

作者：Yu Zhang, Tia S. Lee, Joseph M. Favale, Dylan C. Leary, Jeffrey L. Petersen, Gregory D. Scholes, Felix N. Castellano & Carsten Milsmann

摘要：Advances in chemical control of the photophysical properties of transition-metal complexes are revolutionizing a wide range of technologies, particularly photocatalysis and light-emitting diodes, but they rely heavily on molecules containing precious metals such as ruthenium and iridium. Although the application of earth-abundant 'early' transition metals in photosensitizers is clearly advantageous, a detailed understanding of excited states with ligand-to-metal charge transfer (LMCT) character is paramount to account for their distinct electron configurations. Here we report an air- and moisture-stable, visible light-absorbing Zr(IV) photosensitizer, Zr(MesPDPPh)2, where [MesPDPPh]2− is the doubly deprotonated form of [2,6-bis(5-(2,4,6-trimethylphenyl)-3-phenyl-1H-pyrrol-2-yl)pyridine]. This molecule has an exceptionally long-lived triplet LMCT excited state ($\tau = 350\,\mu s$), featuring highly efficient photoluminescence emission ($\Phi = 0.45$) due to thermally activated delayed fluorescence emanating from the higher-lying singlet configuration with significant LMCT contributions. Zr(MesPDPPh)2 engages in numerous photoredox catalytic processes and triplet energy transfer. Our investigation provides a blueprint for future photosensitizer development featuring early transition metals and excited states with significant LMCT contributions.

链接：https://www.nature.com/articles/s41557-020-0430-7

10. **标题：** The merger of decatungstate and copper catalysis to enable aliphatic C(sp3)–H trifluoromethylation

作者：Patrick J. Sarver, Vlad Bacauanu, Danielle M. Schultz, Daniel A. DiRocco, Yu-hong Lam, Edward C. Sherer & David W. C. MacMillan

摘要：The introduction of a trifluoromethyl (CF3) group can dramatically improve a compound's biological properties. Despite the well-established importance of trifluoromethylated compounds, general methods for the trifluoromethylation of alkyl C–H bonds remain elusive. Here we report the development of a dual-catalytic C(sp3)–H trifluoromethylation through the merger of light-driven,

decatungstate-catalysed hydrogen atom transfer and copper catalysis. This metallaphotoredox methodology enables the direct conversion of both strong aliphatic and benzylic C–H bonds into the corresponding C(sp3)–CF3 products in a single step using a bench-stable, commercially available trifluoromethylation reagent. The reaction requires only a single equivalent of substrate and proceeds with excellent selectivity for positions distal to unprotected amines. To demonstrate the utility of this new methodology for late-stage functionalization, we have directly derivatized a broad range of approved drugs and natural products to generate valuable trifluoromethylated analogues. Preliminary mechanistic experiments reveal that a 'Cu–CF3' species is formed during this process and the critical C(sp3)–CF3 bond-forming step involves the copper catalyst.

链接：https://www.nature.com/articles/s41557-020-0436-1

11.**标题：**A photoswitchable polar crystal that exhibits superionic conduction

作者：Shin-ichi Ohkoshi, Kosuke Nakagawa, Kenta Imoto, Hiroko Tokoro, Yuya Shibata, Kohei Okamoto, Yasuto Miyamoto, Masaya Komine, Marie Yoshikiyo & Asuka Namai

摘要：Ionic conductors serve as solid electrolytes for fuel cells and batteries, whereas polar crystals such as ferroelectrics and pyroelectrics—which are typically insulating materials—are used in electronic devices. Here we show a material that combines superionic conductivity with a polar crystal structure at room temperature. This three-dimensional anionic network is based on －Fe－N≡C－Mo－ units, with Cs cations hosted in every other pore. In the resulting $Cs_{1.1}Fe_{0.95}[Mo(CN)_5(NO)] \cdot 4H_2O$ material, the negative and positive charges of the framework and Cs+ ions, respectively, are non-symmetrically shifted in the c-axis direction of the unit cell, and spontaneous electric polarization is generated, in turn leading to second harmonic generation (SHG). Additionally, this material is a superionic conductor (with an ionic conductivity value of 4×10^{-3} S cm−1 at 318 K). Furthermore, the ionic conductivity significantly decreases under 532 nm light irradiation (from 1×10^{-3} S cm−1 to 6×10^{-5} S cm−1 at room temperature) and, when irradiation stops, returns to its original value within ~1 h.

链接：https://www.nature.com/articles/s41557-020-0427-2

12.**标题：**A programmable polymer library that enables the construction of stimuli-responsive nanocarriers containing logic gates

作者：Penghui Zhang, Di Gao, Keli An, Qi Shen, Chen Wang, Yuchao Zhang, Xiaoshu Pan, Xigao Chen, Yifan Lyv, Cheng Cui, Tingxizi Liang, Xiaoman Duan, Jie Liu, Tielin Yang, Xiaoxiao Hu, Jun-Jie Zhu, Feng Xu & Weihong Tan

摘要：Stimuli-responsive biomaterials that contain logic gates hold great potential for detecting and responding to pathological markers as part of clinical therapies. However, a major barrier is the lack of a generalized system that can be used to easily assemble different ligand-responsive units to form programmable nanodevices for advanced biocomputation. Here we develop a programmable polymer library by including responsive units in building blocks with similar structure and reactivity. Using these polymers, we have developed a series of smart nanocarriers with hierarchical structures containing logic gates linked to self-immolative motifs. Designed with disease biomarkers as inputs, our logic devices showed site-specific release of multiple therapeutics (including kinase inhibitors, drugs and short interfering RNA) in vitro and in vivo. We expect that this 'plug and play' platform will be expanded towards smart biomaterial engineering for therapeutic delivery, precision medicine,

tissue engineering and stem cell therapy.
链接：https://www.nature.com/articles/s41557-020-0426-3

13.**标题：**Connecting remote C–H bond functionalization and decarboxylative coupling using simple amines
作者：Francisco de Azambuja, Ming-Hsiu Yang, Taisiia Feoktistova, Manikandan Selvaraju, Alexander C. Brueckner, Markas A. Grove, Suvajit Koley, Paul Ha-Yeon Cheong & Ryan A. Altman
摘要：Transition metal-catalysed C–H functionalization and decarboxylative coupling are two of the most notable synthetic strategies developed in the past 30 years. Here, we connect these two reaction pathways using bases and a simple Pd-based catalyst system to promote a para-selective C–H functionalization reaction from benzylic electrophiles. Experimental and computational mechanistic studies suggest a pathway that involves an uncommon Pd-catalysed dearomatization of the benzyl moiety followed by a base-enabled rearomatization through a formal 1,5-hydrogen migration. This reaction complements ‘C–H activation’ strategies that convert inert C–H bonds into C–metal bonds prior to C–C bond formation. Instead, this reaction exploits an inverted sequence and promotes C–C bond formation prior to deprotonation. These studies provide an opportunity to develop general para-selective C–H functionalization reactions from benzylic electrophiles and show how new reactive modalities may be accessed with careful control of the reaction conditions.
链接：https://www.nature.com/articles/s41557-020-0428-1

14.**标题:** Odd–even alternations in helical propensity of a homologous series of hydrocarbons
作者：Johan A. Pradeilles, Siying Zhong, Márton Baglyas, György Tarczay, Craig P. Butts, Eddie L. Myers & Varinder K. Aggarwal
摘要：Odd and even homologues of some n-alkane-based systems are known to exhibit notably different trends in solid-state properties; a well-known illustration is the zigzag plot of their melting point versus chain length. Odd–even effects in the solid state often arise from intermolecular interactions that involve fully extended molecules. These effects have also been observed in less condensed phases, such as self-assembled monolayers; however, the origins of these effects in such systems can be difficult to determine. Here we combined NMR and computational analysis to show that all-syn contiguously methyl-substituted hydrocarbons, with chain lengths from C6 to C11, exhibit a dramatic odd–even effect in helical propensity. The even- and odd-numbered hydrocarbons populate regular and less-controlled helical conformations, respectively. This knowledge will guide the design of helical hydrocarbons as rigid scaffolds or as hydrophobic components in soft materials.
链接：https://www.nature.com/articles/s41557-020-0429-0

15.**标题：**Differentiation and functionalization of remote C–H bonds in adjacent positions
作者：Hang Shi, Yi Lu, Jiang Weng, Katherine L. Bay, Xiangyang Chen, Keita Tanaka, Pritha Verma, Kendall N. Houk & Jin-Quan Yu
摘要：Site-selective functionalization of C–H bonds will ultimately afford chemists transformative tools for editing and constructing complex molecular architectures. Towards this goal, it is essential to develop strategies to activate C–H bonds that are distal from a functional group. In this context, distinguishing remote C–H bonds on adjacent carbon atoms is an extraordinary challenge due to the lack of electronic or steric bias between the two positions. Herein, we report the design of a catalytic

system leveraging a remote directing template and a transient norbornene mediator to selectively activate a previously inaccessible remote C–H bond that is one bond further away. The generality of this approach has been demonstrated with a range of heterocycles, including a complex anti-leukaemia agent and hydrocinnamic acid substrates.

链接：https://www.nature.com/articles/s41557-020-0424-5

16. **标 题 ：** Vibrational coherences in manganese single-molecule magnets after ultrafast photoexcitation

作者：Florian Liedy, Julien Eng, Robbie McNab, Ross Inglis, Thomas J. Penfold, Euan K. Brechin & J. Olof Johansson

摘要：Magnetic recording using femtosecond laser pulses has recently been achieved in some dielectric media, showing potential for ultrafast data storage applications. Single-molecule magnets (SMMs) are metal complexes with two degenerate magnetic ground states and are promising for increasing storage density, but remain unexplored using ultrafast techniques. Here we have explored the dynamics occurring after photoexcitation of a trinuclear μ3-oxo-bridged Mn(III)-based SMM, whose magnetic anisotropy is closely related to the Jahn–Teller distortion. Ultrafast transient absorption spectroscopy in solution reveals oscillations superimposed on the decay traces due to a vibrational wavepacket. Based on complementary measurements and calculations on the monomer Mn(acac)3, we conclude that the wavepacket motion in the trinuclear SMM is constrained along the Jahn–Teller axis due to the μ3-oxo and μ-oxime bridges. Our results provide new possibilities for optical control of the magnetization in SMMs on femtosecond timescales and open up new molecular-design challenges to control the wavepacket motion in the excited state of polynuclear transition-metal complexes.

链接：https://www.nature.com/articles/s41557-020-0431-6

17.**标题：**Spatial separation of triplet excitons drives endothermic singlet fission

作者：Nadezhda V. Korovina, Christopher H. Chang & Justin C. Johnson

摘要：Molecules that undergo singlet fission, converting singlet excitons into pairs of triplet excitons, have potential as photovoltaic materials. The possible advantages of endothermic singlet fission (enhanced use of photon energy and larger triplet energies for coupling with common absorbers) motivated us to assess the role of exciton delocalization in the activation of this process. Here we report the synthesis of a series of linear perylene oligomers that undergo endothermic singlet fission and have endothermicities in the range 5–10 kBT at room temperature in solution. We study these compounds using transient spectroscopy and modelling to unravel the singlet and triplet dynamics. We show that the minimal number of coupled chromophores needed to undergo endothermic singlet fission is three, which provides sufficient statistical space for triplet excitons to separate and avoid annihilation—and a subsequent fast return to the singlet state. Our data additionally suggest that torsional motion of chromophores about the molecular axis following triplet-pair separation contributes to the increase in entropy, thus lengthening the triplet lifetime in longer oligomers.

链接：https://www.nature.com/articles/s41557-020-0422-7

18.**标题：**Heteromeric three-stranded coiled coils designed using a Pb(II)(Cys)3 template mediated strategy

作者：Audrey E. Tolbert, Catherine S. Ervin, Leela Ruckthong, Thomas J. Paul, Vindi M. Jayasinghe-Arachchige, Kosh P. Neupane, Jeanne A. Stuckey, Rajeev Prabhakar & Vincent L. Pecoraro

摘要：Three-stranded coiled coils are peptide structures constructed from amphipathic heptad repeats. Here we show that it is possible to form pure heterotrimeric three-stranded coiled coils by combining three distinct characteristics: (1) a cysteine sulfur layer for metal coordination, (2) a thiophilic, trigonal pyramidal metalloid (Pb(II)) that binds to these sulfurs and (3) an adjacent layer of reduced steric bulk generating a cavity where water can hydrogen bond to the cysteine sulfur atoms. Cysteine substitution in an a site yields Pb(II)A2B heterotrimers, while d sites provide pure Pb(II)C2D or Pb(II)CD2 scaffolds. Altering the metal from Pb(II) to Hg(II) or shifting the relative position of the sterically less demanding layer removes heterotrimer specificity. Because only two of the eight or ten hydrophobic layers are perturbed, catalytic sites can be introduced at other regions of the scaffold. A Zn(II)(histidine)3(H2O) centre can be incorporated at a remote location without perturbing the heterotrimer selectivity, suggesting a unique strategy to prepare dissymmetric catalytic sites within self-assembling de novo-designed proteins.

链接：https://www.nature.com/articles/s41557-020-0423-6

19.**标题：**Modular bismacycles for the selective C–H arylation of phenols and naphthols

作者：Mark Jurrat, Lorenzo Maggi, William Lewis & Liam T. Ball

摘要：Given the important role played by 2-hydroxybiaryls in organic, medicinal and materials chemistry, concise methods for the synthesis of this common motif are extremely valuable. In seeking to extend the lexicon of synthetic chemists in this regard, we have developed an expedient and general strategy for the ortho-arylation of phenols and naphthols using readily available boronic acids. Our methodology relies on in situ generation of a uniquely reactive Bi(V) arylating agent from a bench-stable Bi(III) precursor via telescoped B–to–Bi transmetallation and oxidation. By exploiting reactivity that is orthogonal to conventional metal-catalysed manifolds, diverse aryl and heteroaryl partners can be rapidly coupled to phenols and naphthols under mild conditions. Following arylation, high-yielding recovery of the Bi(III) precursor allows for its efficient re-use in subsequent reactions. Mechanistic interrogation of each key step of the methodology informs its practical application and provides fundamental insight into the underexploited reactivity of organobismuth compounds.

链接：https://www.nature.com/articles/s41557-020-0425-4

20.**标题：**Author Correction: Ruthenium-catalysed oxidative conversion of ammonia into dinitrogen

作者：Kazunari Nakajima, Hiroki Toda, Ken Sakata & Yoshiaki Nishibayashi

摘要：In the version of this Article originally published, the last sentence of the first paragraph incorrectly read: ‘However, to the best of our knowledge, catalytic conversion of ammonia into dinitrogen with transition metal complexes has not yet been achieved7, although several groups have reported stoichiometric reactivities of transition metal–ammonia complexes with oxidative electron transfer8–10 and hydrogen atom abstraction conditions11–13.

This sentence has been corrected to read as follows: ‘During the review process for this manuscript, Hamann, Smith and co-workers reported the ability of ruthenium polypyridyl complexes to catalyse

ammonia oxidation to dinitrogen7. Aside from this work, to the best of our knowledge, there are no other reports on the catalytic conversion of ammonia into dinitrogen with transition metal complexes, although several groups have reported stoichiometric reactivities of transition metal–ammonia complexes with oxidative electron transfer8–10 and hydrogen atom abstraction conditions11–13.'

链接：https://www.nature.com/articles/s41557-020-0441-4

21. **标 题 ：** Interface-mediated noble metal deposition on transition metal dichalcogenide nanostructures

作者：Yifan Sun, Yuanxi Wang, Jamie Y. C. Chen, Kazunori Fujisawa, Cameron F. Holder, Jeffery T. Miller, Vincent H. Crespi, Mauricio Terrones & Raymond E. Schaak

摘要：Functionalizing the surfaces of transition metal dichalcogenide (TMD) nanosheets with noble metals is important for electrically contacting them to devices, as well as improving their catalytic and sensing capabilities. Solution-phase deposition provides a scalable approach to the creation of metal–TMD hybrid systems, but controlling such processes remains challenging. Here we elucidate the different pathways by which gold and silver deposit at room temperature onto colloidal 1T-WS2, 2H-WS2, 2H-MoSe2, 2H-WSe2, 1T′ -MoTe2 and Td-WTe2 few-layer nanostructures to produce several distinct classes of 0D – 2D and 2D – 2D metal – TMD hybrids. Uniform gold nanoparticles form on all of the TMDs. By contrast, silver deposits as nanoparticles with a bimodal size distribution on the disulfides and diselenides, and as atomically thin layers on the ditellurides. The various sizes and morphologies of these surface-bound metal species arise from the relative strengths of the interfacial metal–chalcogen bonds during the reduction of Au3+ or Ag+ by the TMDs.

链接：https://www.nature.com/articles/s41557-020-0418-3

22. **标题：**Coordination cages as permanently porous ionic liquids

作者：Lillian Ma, Cally J. E. Haynes, Angela B. Grommet, Anna Walczak, Christopher C. Parkins, Cara M. Doherty, Louis Longley, Arnaud Tron, Artur R. Stefankiewicz, Thomas D. Bennett & Jonathan R. Nitschke

摘要：Porous materials are widely used in industry for applications that include chemical separations and gas scrubbing. These materials are typically porous solids, although the liquid state can be easier to manipulate in industrial settings. The idea of combining the size and shape selectivity of porous domains with the fluidity of liquids is a promising one and porous liquids composed of functionalized organic cages have recently attracted attention. Here we describe an ionic-liquid, porous, tetrahedral coordination cage. Complementing the gas binding observed in other porous liquids, this material also encapsulates non-gaseous guests—shape and size selectivity was observed for a series of isomeric alcohols. Three gaseous chlorofluorocarbon guests, trichlorofluoromethane, dichlorodifluoromethane and chlorotrifluoromethane, were also shown to be taken up by the liquid coordination cage with an affinity that increased with their size. We hope that these findings will lead to the synthesis of other porous liquids whose guest-uptake properties may be tailored to fulfil specific functions.

链接：https://www.nature.com/articles/s41557-020-0419-2

23. **标题：**Electronic complementarity permits hindered butenolide heterodimerization and discovery of novel cGAS/STING pathway antagonists

作者：Benjamin J. Huffman, Shuming Chen, J. Luca Schwarz, R. Erik Plata, Emily N. Chin, Luke L. Lairson, K. N. Houk & Ryan A. Shenvi

摘要：sp3-hybridized attached-rings are common motifs in secondary metabolites and represent tetrahedral equivalents to the biaryl substructures that overpopulate synthetic libraries. Few methods are available that can link fully substituted carbon atoms of two rings with stereocontrol. Here we have developed a stereoselective, heteroselective butenolide coupling that exhibits an unusually fast rate of C–C bond formation driven by exquisite complementarity of the reacting π systems. Heterodimerization generates a compound collection with topological complexity and diverse principal moments of inertia. The special status of the sp3–sp3 attached-ring motif is demonstrated in a high-throughput screen for inhibitors of the cyclic GMP-AMP synthase/stimulator of interferon genes pathway, which recruited these butenolide heterodimers from a field of 250,000 compounds. The driving forces underlying this general attached-ring coupling identify a novel paradigm for the accession of wider natural product chemical space, accelerating the discovery of selective lead compounds.

链接：https://www.nature.com/articles/s41557-019-0413-8

24. **标题：**Nickel-catalysed anti-Markovnikov hydroarylation of unactivated alkenes with unactivated arenes facilitated by non-covalent interactions

作者：Noam I. Saper, Akito Ohgi, David W. Small, Kazuhiko Semba, Yoshiaki Nakao & John F. Hartwig

摘要：Anti-Markovnikov additions to alkenes have been a longstanding goal of catalysis, and anti-Markovnikov addition of arenes to alkenes would produce alkylarenes that are distinct from those formed by acid-catalysed processes. Existing hydroarylations are either directed or occur with low reactivity and low regioselectivity for the n-alkylarene. Herein, we report the first undirected hydroarylation of unactivated alkenes with unactivated arenes that occurs with high regioselectivity for the anti-Markovnikov product. The reaction occurs with a nickel catalyst ligated by a highly sterically hindered N-heterocyclic carbene. Catalytically relevant arene- and alkene-bound nickel complexes have been characterized, and the rate-limiting step was shown to be reductive elimination to form the C–C bond. Density functional theory calculations, combined with second-generation absolutely localized molecular orbital energy decomposition analysis, suggest that the difference in activity between catalysts containing large and small carbenes results more from stabilizing intramolecular non-covalent interactions in the secondary coordination sphere than from steric hindrance.

链接：https://www.nature.com/articles/s41557-019-0409-4

25. **标题：**Proteomimetics as protein-inspired scaffolds with defined tertiary folding patterns

作者：W. Seth Horne & Tom N. Grossmann

摘要：Proteins have evolved as a variable platform that provides access to molecules with diverse shapes, sizes and functions. These features have inspired chemists for decades to seek artificial mimetics of proteins with improved or novel properties. Such work has focused primarily on small protein fragments, often isolated secondary structures; however, there has lately been a growing

interest in the design of artificial molecules that mimic larger, more complex tertiary folds. In this Perspective, we define these agents as ‘proteomimetics’ and discuss the recent advances in the field. Proteomimetics can be divided into three categories: protein domains with side-chain functionality that alters the native linear-chain topology; protein domains in which the chemical composition of the polypeptide backbone has been partially altered; and protein-like folded architectures that are composed entirely of non-natural monomer units. We give an overview of these proteomimetic approaches and outline remaining challenges facing the field.

链接：https://www.nature.com/articles/s41557-020-0420-9

IEL Top25

（来源：http://ieeexplore.ieee.org/）

1.标题：Change Management Models: A Comparative Analysis and Concerns
出处：IEEE Engineering Management Review (Volume: 46 , Issue: 3 , thirdquarter,Sept. 1 2018
作者：Brian Joseph Galli
摘要：To better understand change management, we compare some popular change management models in relation to project management and organizations in this study. After a brief introduction of five major models, various advantages and disadvantages are identified for each. Lessons and implications for organizations and management are also introduced
链接：https://ieeexplore.ieee.org/document/8486843

2.标题：Efficient Epileptic Seizure Prediction Based on Deep Learning
出处：IEEE Transactions on Biomedical Circuits and Systems
作者：Hisham Daoud ; Magdy A. Bayoumi
摘要：Epilepsy is one of the world's most common neurological diseases. Early prediction of the incoming seizures has a great influence on epileptic patients' life. In this paper, a novel patient-specific seizure prediction technique based on deep learning and applied to long-term scalp electroencephalogram (EEG) recordings is proposed. The goal is to accurately detect the preictal brain state and differentiate it from the prevailing interictal state as early as possible and make it suitable for real time. The features extraction and classification processes are combined into a single automated system. Raw EEG signal without any preprocessing is considered as the input to the system which further reduces the computations. Four deep learning models are proposed to extract the most discriminative features which enhance the classification accuracy and prediction time. The proposed approach takes advantage of the convolutional neural network in extracting the significant spatial features from different scalp positions and the recurrent neural network in expecting the incidence of seizures earlier than the current methods. A semi-supervised approach based on transfer learning technique is introduced to improve the optimization problem. A channel selection algorithm is proposed to select the most relevant EEG channels which makes the proposed system good candidate for real-time usage. An effective test method is utilized to ensure robustness. The achieved highest accuracy of 99.6% and lowest false alarm rate of 0.004 h - 1 along with very early seizure prediction time of 1 h make the proposed method the most efficient among the state of the art.
链接：https://ieeexplore.ieee.org/document/8765420

3.标题：Improving Pedestrian Safety in Cities Using Intelligent Wearable Systems
出处：IEEE Internet of Things Journal
作者：Stephen Xia ; Daniel de Godoy Peixoto ; Bashima Islam ; Md Tamzeed Islam ; Shahriar Nirjon ; Peter R. Kinget ; Xiaofan Jiang
摘要：With the prevalence of smartphones, pedestrians and joggers today often walk or run while

listening to music. Since they are deprived of their auditory senses that would have provided important cues to dangers, they are at a much greater risk of being hit by cars or other vehicles. In this paper, we build a wearable system that uses multichannel audio sensors embedded in a headset to help detect and locate cars from their honks, engine, and tire noises, and warn pedestrians of imminent dangers of approaching cars. We demonstrate that using a segmented architecture consisting of headset-mounted audio sensors, a front-end hardware platform that performs signal processing and feature extraction, and machine learning-based classification on a smartphone, we are able to provide early danger detection in real time, from up to 60 m away, and alert the user with low latency and high accuracy. To further reduce power consumption of the battery-powered wearable headset, we implement a custom-designed integrated circuit that is able to compute delays between multiple channels of audio with nW power consumption. A regression-based method for sound source localization, angle via polygonal regression, is proposed and used in combination with the IC to improve the granularity and robustness of localization.
链接：https://ieeexplore.ieee.org/document/8662658

4.标题：6Genesis Flagship Program: Building the Bridges Towards 6G-Enabled Wireless Smart Society and Ecosystem
出处：2018 IEEE 10th Latin-American Conference on Communications (LATINCOM)
作者：Marcos Katz ; Marja Matinmikko-Blue ; Matti Latva-Aho
摘要：In this paper, an initial vision of what the sixth generation mobile communication system (6G)might be is presented. This is done through the primary ideas of the 6Genesis Flagship Program (6GFP), a recently formed Finnish academic and industrial consortium aiming at developing key enabling technologies for 6G. 6GFP is an eight-year large-scale research initiative set to ultimately develop, implement and test key enabling technologies for 6G. Motivations, visions, trends and expectations for 6G are first discussed to set the ground for further development. Four main research areas are proposed as the starting point, encompassing not only wireless communications but also computer science, electronics and material science as well as applications and services. The paper provides an in-detail list of technical topics going to be studied in this program, and in general, worth considering for everyone planning to develop beyond 5G technology. The paper also shed some light on how the research will be implemented, showing the logic and relationships between the research areas, discussing already selected promising enabling technology for 6G, as well as envisioning how the proof-of-concept of the developed system will be carried out. An existing state-of-the-art 5G network will be used as the starting point for developing and testing the novel concepts and technologies created in the program.
链接：https://ieeexplore.ieee.org/document/8613209

5.标题：Review of Deep Learning Algorithms and Architectures
出处：IEEE Access (Volume: 7)
作者：Ajay Shrestha ; Ausif Mahmood
摘要：Deep learning (DL) is playing an increasingly important role in our lives. It has already made a huge impact in areas, such as cancer diagnosis, precision medicine, self-driving cars, predictive forecasting, and speech recognition. The painstakingly handcrafted feature extractors used in traditional learning, classification, and pattern recognition systems are not scalable for large-sized

data sets. In many cases, depending on the problem complexity, DL can also overcome the limitations of earlier shallow networks that prevented efficient training and abstractions of hierarchical representations of multi-dimensional training data. Deep neural network (DNN) uses multiple (deep) layers of units with highly optimized algorithms and architectures. This paper reviews several optimization methods to improve the accuracy of the training and to reduce training time. We delve into the math behind training algorithms used in recent deep networks. We describe current shortcomings, enhancements, and implementations. The review also covers different types of deep architectures, such as deep convolution networks, deep residual networks, recurrent neural networks, reinforcement learning, variational autoencoders, and others.
链接：https://ieeexplore.ieee.org/document/8694781

6.标题：Internet of Things: A Comprehensive Study of Security Issues and Defense Mechanisms 出处：IEEE Access (Volume: 7)
作者：Tariq Ahamed Ahanger ; Abdullah Aljumah
摘要：The Internet of Things (IoT) is an evolving global trend in Web-based information architecture aiding in the exchange of services and goods over a network without necessitating human-to-human or human-to-computer interaction. It has the potential to revolutionize physical world interaction of individuals and the organizations. The application of IoT can be recognized significantly in many areas such as in healthcare, resource management, learning, knowledge processing, and many more. The practical realization of IoT is met with a plethora of security and privacy challenges that need to be tackled for IoT's successful deployment on a commercially viable large scale. This paper analyzes the security issues related to IoT networks through an analysis of the existing empirical researches to get an insight on the security requirements of the IoT networks. The findings of the study revealed that security threats are one of the biggest and ever-growing challenges for IoT, and it is essential to substantially mitigate them for the success of this platform.
链接：https://ieeexplore.ieee.org/document/8519613

7.标题：Learning Robust Control Policies for End-to-End Autonomous Driving From Data-Driven Simulation
出处：IEEE Access (Volume: 7)
作者：Alexander Amini ; Igor Gilitschenski ; Jacob Phillips ; Julia Moseyko ; Rohan Banerjee ; Sertac Karaman ; Daniela Rus
摘要：In this work, we present a data-driven simulation and training engine capable of learning end-to-end autonomous vehicle control policies using only sparse rewards. By leveraging real, human-collected trajectories through an environment, we render novel training data that allows virtual agents to drive along a continuum of new local trajectories consistent with the road appearance and semantics, each with a different view of the scene. We demonstrate the ability of policies learned within our simulator to generalize to and navigate in previously unseen real-world roads, without access to any human control labels during training. Our results validate the learned policy onboard a full-scale autonomous vehicle, including in previously un-encountered scenarios, such as new roads and novel, complex, near-crash situations. Our methods are scalable, leverage reinforcement learning, and apply broadly to situations requiring effective perception and robust operation in the physical world.

链接：https://ieeexplore.ieee.org/document/8957584

8.标题：Peeking Inside the Black-Box: A Survey on Explainable Artificial Intelligence (XAI)
出处：IEEE Access (Volume: 6)
作者：Amina Adadi ; Mohammed Berrada
摘要：At the dawn of the fourth industrial revolution, we are witnessing a fast and widespread adoption of artificial intelligence (AI) in our daily life, which contributes to accelerating the shift towards a more algorithmic society. However, even with such unprecedented advancements, a key impediment to the use of AI-based systems is that they often lack transparency. Indeed, the black-box nature of these systems allows powerful predictions, but it cannot be directly explained. This issue has triggered a new debate on explainable AI (XAI). A research field holds substantial promise for improving trust and transparency of AI-based systems. It is recognized as the sine qua non for AI to continue making steady progress without disruption. This survey provides an entry point for interested researchers and practitioners to learn key aspects of the young and rapidly growing body of research related to XAI. Through the lens of the literature, we review the existing approaches regarding the topic, discuss trends surrounding its sphere, and present major research trajectories.
链接：https://ieeexplore.ieee.org/document/8466590

9.标题：A Survey of Data Mining and Machine Learning Methods for Cyber Security Intrusion Detection
出处：IEEE Communications Surveys & Tutorials (Volume: 18 , Issue: 2 , Secondquarter 2016)
作者：Anna L. Buczak ; Erhan Guven
摘要：This survey paper describes a focused literature survey of machine learning (ML) and data mining (DM) methods for cyber analytics in support of intrusion detection. Short tutorial descriptions of each ML/DM method are provided. Based on the number of citations or the relevance of an emerging method, papers representing each method were identified, read, and summarized. Because data are so important in ML/DM approaches, some well-known cyber data sets used in ML/DM are described. The complexity of ML/DM algorithms is addressed, discussion of challenges for using ML/DM for cyber security is presented, and some recommendations on when to use a given method are provided.
链接：https://ieeexplore.ieee.org/document/7307098

10.标题：Deep Learning Applications in Medical Image Analysis
出处：IEEE Access (Volume: 6)
作者：Justin Ker ; Lipo Wang ; Jai Rao ; Tchoyoson Lim
摘要：The tremendous success of machine learning algorithms at image recognition tasks in recent years intersects with a time of dramatically increased use of electronic medical records and diagnostic imaging. This review introduces the machine learning algorithms as applied to medical image analysis, focusing on convolutional neural networks, and emphasizing clinical aspects of the field. The advantage of machine learning in an era of medical big data is that significant hierarchal relationships within the data can be discovered algorithmically without laborious hand-crafting of features. We cover key research areas and applications of medical image classification, localization, detection, segmentation, and registration. We conclude by discussing research obstacles, emerging

trends, and possible future directions.
链接：https://ieeexplore.ieee.org/document/8241753

11.标题：Disease Prediction by Machine Learning Over Big Data From Healthcare Communities 出处：IEEE Access (Volume: 5)
作者：Min Chen ; Yixue Hao ; Kai Hwang ; Lu Wang ; Lin Wang
摘要：With big data growth in biomedical and healthcare communities, accurate analysis of medical data benefits early disease detection, patient care, and community services. However, the analysis accuracy is reduced when the quality of medical data is incomplete. Moreover, different regions exhibit unique characteristics of certain regional diseases, which may weaken the prediction of disease outbreaks. In this paper, we streamline machine learning algorithms for effective prediction of chronic disease outbreak in disease-frequent communities. We experiment the modified prediction models over real-life hospital data collected from central China in 2013-2015. To overcome the difficulty of incomplete data, we use a latent factor model to reconstruct the missing data. We experiment on a regional chronic disease of cerebral infarction. We propose a new convolutional neural network (CNN)-based multimodal disease risk prediction algorithm using structured and unstructured data from hospital. To the best of our knowledge, none of the existing work focused on both data types in the area of medical big data analytics. Compared with several typical prediction algorithms, the prediction accuracy of our proposed algorithm reaches 94.8% with a convergence speed, which is faster than that of the CNN-based unimodal disease risk prediction algorithm.
链接：https://ieeexplore.ieee.org/document/7912315

12.标题：A Survey of 5G Network: Architecture and Emerging Technologies
出处：IEEE Access (Volume: 3)
作者：A. Gupta ; R. K. Jha
摘要：In the near future, i.e., beyond 4G, some of the prime objectives or demands that need to be addressed are increased capacity, improved data rate, decreased latency, and better quality of service. To meet these demands, drastic improvements need to be made in cellular network architecture. This paper presents the results of a detailed survey on the fifth generation (5G) cellular network architecture and some of the key emerging technologies that are helpful in improving the architecture and meeting the demands of users. In this detailed survey, the prime focus is on the 5G cellular network architecture, massive multiple input multiple output technology, and device-to-device communication (D2D). Along with this, some of the emerging technologies that are addressed in this paper include interference management, spectrum sharing with cognitive radio, ultra-dense networks, multi-radio access technology association, full duplex radios, millimeter wave solutions for 5G cellular networks, and cloud technologies for 5G radio access networks and software defined networks. In this paper, a general probable 5G cellular network architecture is proposed, which shows that D2D, small cell access points, network cloud, and the Internet of Things can be a part of 5G cellular network architecture. A detailed survey is included regarding current research projects being conducted in different countries by research groups and institutions that are working on 5G technologies.
链接：https://ieeexplore.ieee.org/document/7169508

13.标题：Internet-of-Things (IoT)-Based Smart Agriculture: Toward Making the Fields Talk
出处：IEEE Access (Volume: 7)
作者：Muhammad Ayaz ; Mohammad Ammad-Uddin ; Zubair Sharif ; Ali Mansour ; El-Hadi M. Aggoune
摘要：Despite the perception people may have regarding the agricultural process, the reality is that today's agriculture industry is data-centered, precise, and smarter than ever. The rapid emergence of the Internet-of-Things (IoT) based technologies redesigned almost every industry including “smart agriculture” which moved the industry from statistical to quantitative approaches. Such revolutionary changes are shaking the existing agriculture methods and creating new opportunities along a range of challenges. This article highlights the potential of wireless sensors and IoT in agriculture, as well as the challenges expected to be faced when integrating this technology with the traditional farming practices. IoT devices and communication techniques associated with wireless sensors encountered in agriculture applications are analyzed in detail. What sensors are available for specific agriculture application, like soil preparation, crop status, irrigation, insect and pest detection are listed. How this technology helping the growers throughout the crop stages, from sowing until harvesting, packing and transportation is explained. Furthermore, the use of unmanned aerial vehicles for crop surveillance and other favorable applications such as optimizing crop yield is considered in this article. State-of-the-art IoT-based architectures and platforms used in agriculture are also highlighted wherever suitable. Finally, based on this thorough review, we identify current and future trends of IoT in agriculture and highlight potential research challenges.
链接：https://ieeexplore.ieee.org/document/8784034

14.标题：The Internet of Things for Health Care: A Comprehensive Survey
出处：IEEE Access (Volume: 3)
作者：S. M. Riazul Islam ; Daehan Kwak ; MD. Humaun Kabir ; Mahmud Hossain ; Kyung-Sup Kwak
摘要：The Internet of Things (IoT) makes smart objects the ultimate building blocks in the development of cyber-physical smart pervasive frameworks. The IoT has a variety of application domains, including health care. The IoT revolution is redesigning modern health care with promising technological, economic, and social prospects. This paper surveys advances in IoT-based health care technologies and reviews the state-of-the-art network architectures/platforms, applications, and industrial trends in IoT-based health care solutions. In addition, this paper analyzes distinct IoT security and privacy features, including security requirements, threat models, and attack taxonomies from the health care perspective. Further, this paper proposes an intelligent collaborative security model to minimize security risk; discusses how different innovations such as big data, ambient intelligence, and wearables can be leveraged in a health care context; addresses various IoT and eHealth policies and regulations across the world to determine how they can facilitate economies and societies in terms of sustainable development; and provides some avenues for future research on IoT-based health care based on a set of open issues and challenges.
链接：https://ieeexplore.ieee.org/document/7113786

15.标题：Millimeter Wave Mobile Communications for 5G Cellular: It Will Work!
出处：IEEE Access (Volume: 1)
作者：Theodore S. Rappaport ; Shu Sun ; Rimma Mayzus ; Hang Zhao ; Yaniv Azar ; Kevin Wang ; George N. Wong ; Jocelyn K. Schulz ; Mathew Samimi ; Felix Gutierrez
摘要：The global bandwidth shortage facing wireless carriers has motivated the exploration of the underutilized millimeter wave (mm-wave) frequency spectrum for future broadband cellular communication networks. There is, however, little knowledge about cellular mm-wave propagation in densely populated indoor and outdoor environments. Obtaining this information is vital for the design and operation of future fifth generation cellular networks that use the mm-wave spectrum. In this paper, we present the motivation for new mm-wave cellular systems, methodology, and hardware for measurements and offer a variety of measurement results that show 28 and 38 GHz frequencies can be used when employing steerable directional antennas at base stations and mobile devices.
链接：https://ieeexplore.ieee.org/document/6515173/

16.标题：VINS-Mono: A Robust and Versatile Monocular Visual-Inertial State Estimator
出处：IEEE Transactions on Robotics (Volume: 34 , Issue: 4 , Aug. 2018)
作者：Tong Qin ; Peiliang Li ; Shaojie Shen
摘要：One camera and one low-cost inertial measurement unit (IMU) form a monocular visual-inertial system (VINS), which is the minimum sensor suite (in size, weight, and power) for the metric six degrees-of-freedom (DOF) state estimation. In this paper, we present VINS-Mono: a robust and versatile monocular visual-inertial state estimator. Our approach starts with a robust procedure for estimator initialization. A tightly coupled, nonlinear optimization-based method is used to obtain highly accurate visual-inertial odometry by fusing preintegrated IMU measurements and feature observations. A loop detection module, in combination with our tightly coupled formulation, enables relocalization with minimum computation. We additionally perform 4-DOF pose graph optimization to enforce the global consistency. Furthermore, the proposed system can reuse a map by saving and loading it in an efficient way. The current and previous maps can be merged together by the global pose graph optimization. We validate the performance of our system on public datasets and real-world experiments and compare against other state-of-the-art algorithms. We also perform an onboard closed-loop autonomous flight on the microaerial-vehicle platform and port the algorithm to an iOS-based demonstration. We highlight that the proposed work is a reliable, complete, and versatile system that is applicable for different applications that require high accuracy in localization. We open source our implementations for both PCs (https://github.com/HKUST-Aerial-Robotics/VINS-Mono) and iOS mobile devices (https://github.com/HKUST-Aerial-Robotics/VINS-Mobile).
链接：https://ieeexplore.ieee.org/document/8421746

17.标题：Computer Vision and Machine Learning for Viticulture Technology
出处：IEEE Access (Volume: 6)
作者：Kah Phooi Seng ; Li-Minn Ang ; Leigh M. Schmidtke ; Suzy Y. Rogiers
摘要：This paper gives two contributions to the state-of-the-art for viticulture technology research. First, we present a comprehensive review of computer vision, image processing, and machine learning techniques in viticulture. We summarize the latest developments in vision systems and

techniques with examples from various representative studies, including, harvest yield estimation, vineyard management and monitoring, grape disease detection, quality evaluation, and grape phenology. We focus on how computer vision and machine learning techniques can be integrated into current vineyard management and vinification processes to achieve industry relevant outcomes. The second component of the paper presents the new GrapeCS-ML database which consists of images of grape varieties at different stages of development together with the corresponding ground truth data (e.g., pH and Brix) obtained from chemical analysis. One of the objectives of this database is to motivate computer vision and machine learning researchers to develop practical solutions for deployment in smart vineyards. We illustrate the usefulness of the database for a color-based berry detection application for white and red cultivars and give baseline comparisons using various machine learning approaches and color spaces. This paper concludes by highlighting future challenges that need to be addressed prior to successful implementation of this technology in the viticulture industry.
链接：https://ieeexplore.ieee.org/document/8502206

18.标题：A Survey on Transfer Learning
出处：IEEE Transactions on Knowledge and Data Engineering (Volume: 22 , Issue: 10 , Oct. 2010)
作者：Sinno Jialin Pan ; Qiang Yang
摘要：A major assumption in many machine learning and data mining algorithms is that the training and future data must be in the same feature space and have the same distribution. However, in many real-world applications, this assumption may not hold. For example, we sometimes have a classification task in one domain of interest, but we only have sufficient training data in another domain of interest, where the latter data may be in a different feature space or follow a different data distribution. In such cases, knowledge transfer, if done successfully, would greatly improve the performance of learning by avoiding much expensive data-labeling efforts. In recent years, transfer learning has emerged as a new learning framework to address this problem. This survey focuses on categorizing and reviewing the current progress on transfer learning for classification, regression, and clustering problems. In this survey, we discuss the relationship between transfer learning and other related machine learning techniques such as domain adaptation, multitask learning and sample selection bias, as well as covariate shift. We also explore some potential future issues in transfer learning research.
链接：https://ieeexplore.ieee.org/document/5288526

19.标题：Machine Learning and Deep Learning Methods for Cybersecurity
出处：IEEE Access (Volume: 6)
作者：Yang Xin ; Lingshuang Kong ; Zhi Liu ; Yuling Chen ; Yanmiao Li ; Hongliang Zhu ; Mingcheng Gao ; Haixia Hou ; Chunhua Wang
摘要：With the development of the Internet, cyber-attacks are changing rapidly and the cyber security situation is not optimistic. This survey report describes key literature surveys on machine learning (ML) and deep learning (DL) methods for network analysis of intrusion detection and provides a brief tutorial description of each ML/DL method. Papers representing each method were indexed, read, and summarized based on their temporal or thermal correlations. Because data are so important in ML/DL methods, we describe some of the commonly used network datasets used in ML/DL,

discuss the challenges of using ML/DL for cybersecurity and provide suggestions for research directions.

链接：https://ieeexplore.ieee.org/document/8359287

20.标题：Deep Learning for Health Informatics

出处：IEEE Journal of Biomedical and Health Informatics (Volume: 21 , Issue: 1 , Jan. 2017)

作者：Daniele Ravì ; Charence Wong ; Fani Deligianni ; Melissa Berthelot ; Javier Andreu-Perez ; Benny Lo ; Guang-Zhong Yang

摘要：With a massive influx of multimodality data, the role of data analytics in health informatics has grown rapidly in the last decade. This has also prompted increasing interests in the generation of analytical, data driven models based on machine learning in health informatics. Deep learning, a technique with its foundation in artificial neural networks, is emerging in recent years as a powerful tool for machine learning, promising to reshape the future of artificial intelligence. Rapid improvements in computational power, fast data storage, and parallelization have also contributed to the rapid uptake of the technology in addition to its predictive power and ability to generate automatically optimized high-level features and semantic interpretation from the input data. This article presents a comprehensive up-to-date review of research employing deep learning in health informatics, providing a critical analysis of the relative merit, and potential pitfalls of the technique as well as its future outlook. The paper mainly focuses on key applications of deep learning in the fields of translational bioinformatics, medical imaging, pervasive sensing, medical informatics, and public health.

链接：https://ieeexplore.ieee.org/document/7801947

21.标题：Massive MIMO for next generation wireless systems

出处：IEEE Communications Magazine (Volume: 52 , Issue: 2 , February 2014)

作者：Erik G. Larsson ; Ove Edfors ; Fredrik Tufvesson ; Thomas L. Marzetta

摘要：Multi-user MIMO offers big advantages over conventional point-to-point MIMO: it works with cheap single-antenna terminals, a rich scattering environment is not required, and resource allocation is simplified because every active terminal utilizes all of the time-frequency bins. However, multi-user MIMO, as originally envisioned, with roughly equal numbers of service antennas and terminals and frequency-division duplex operation, is not a scalable technology. Massive MIMO (also known as large-scale antenna systems, very large MIMO, hyper MIMO, full-dimension MIMO, and ARGOS) makes a clean break with current practice through the use of a large excess of service antennas over active terminals and time-division duplex operation. Extra antennas help by focusing energy into ever smaller regions of space to bring huge improvements in throughput and radiated energy efficiency. Other benefits of massive MIMO include extensive use of inexpensive low-power components, reduced latency, simplification of the MAC layer, and robustness against intentional jamming. The anticipated throughput depends on the propagation environment providing asymptotically orthogonal channels to the terminals, but so far experiments have not disclosed any limitations in this regard. While massive MIMO renders many traditional research problems irrelevant, it uncovers entirely new problems that urgently need attention: the challenge of making many low-cost low-precision components that work effectively together, acquisition and synchronization for newly joined terminals, the exploitation of extra degrees of freedom provided by

the excess of service antennas, reducing internal power consumption to achieve total energy efficiency reductions, and finding new deployment scenarios. This article presents an overview of the massive MIMO concept and contemporary research on the topic.
链接：https://ieeexplore.ieee.org/document/6736761

22.标题：3D-Printed Liquid Metal Interconnects for Stretchable Electronics
出处：IEEE Sensors Journal (Volume: 19 , Issue: 10 , May15, 15 2019)
作者：Callen Votzke ; Uranbileg Daalkhaijav ; Yiğit Mengüç ; Matthew L. Johnston
摘要：Stretchable electronic circuits and systems will be critical for future wearable devices and smart textiles, where existing flexible printed circuit board techniques severely limit conformal deformation. In this paper, we present a scalable fabrication approach for making robust interconnects for stretchable electronics using 3D-printed liquid metal paste. Direct extrusion of the liquid metal paste eliminates the need for expensive lithographic molds while offering improved conductivity over traditional carbon- and metal-based inks. As a proof of concept, we demonstrate a multi-layer stretchable circuit, including both active and passive electronic components. We additionally present highly stretchable strain sensors, demonstrating stable conductivity of the liquid metal paste circuit interconnects with minimal hysteresis over more than 350 cycles at 200% strain. These two devices are combined to demonstrate a printed stretchable strain sensor with integrated readout circuitry.
链接：https://ieeexplore.ieee.org/document/8624516

23.标题：Toward Scalable Systems for Big Data Analytics: A Technology Tutorial
出处：IEEE Access (Volume: 2)
作者：Han Hu ; Yonggang Wen ; Tat-Seng Chua ; Xuelong Li
摘要：Recent technological advancements have led to a deluge of data from distinctive domains (e.g., health care and scientific sensors, user-generated data, Internet and financial companies, and supply chain systems) over the past two decades. The term big data was coined to capture the meaning of this emerging trend. In addition to its sheer volume, big data also exhibits other unique characteristics as compared with traditional data. For instance, big data is commonly unstructured and require more real-time analysis. This development calls for new system architectures for data acquisition, transmission, storage, and large-scale data processing mechanisms. In this paper, we present a literature survey and system tutorial for big data analytics platforms, aiming to provide an overall picture for nonexpert readers and instill a do-it-yourself spirit for advanced audiences to customize their own big-data solutions. First, we present the definition of big data and discuss big data challenges. Next, we present a systematic framework to decompose big data systems into four sequential modules, namely data generation, data acquisition, data storage, and data analytics. These four modules form a big data value chain. Following that, we present a detailed survey of numerous approaches and mechanisms from research and industry communities. In addition, we present the prevalent Hadoop framework for addressing big data challenges. Finally, we outline several evaluation benchmarks and potential research directions for big data systems.
链接：https://ieeexplore.ieee.org/document/6842585

24.标题：A fast and elitist multiobjective genetic algorithm: NSGA-II
出处：IEEE Transactions on Evolutionary Computation (Volume: 6 , Issue: 2 , Apr 2002)
作者：K. Deb ; A. Pratap ; S. Agarwal ; T. Meyarivan
摘要：Multi-objective evolutionary algorithms (MOEAs) that use non-dominated sorting and sharing have been criticized mainly for: (1) their O(MN/sup 3/) computational complexity (where M is the number of objectives and N is the population size); (2) their non-elitism approach; and (3) the need to specify a sharing parameter. In this paper, we suggest a non-dominated sorting-based MOEA, called NSGA-II (Non-dominated Sorting Genetic Algorithm II), which alleviates all of the above three difficulties. Specifically, a fast non-dominated sorting approach with O(MN/sup 2/) computational complexity is presented. Also, a selection operator is presented that creates a mating pool by combining the parent and offspring populations and selecting the best N solutions (with respect to fitness and spread). Simulation results on difficult test problems show that NSGA-II is able, for most problems, to find a much better spread of solutions and better convergence near the true Pareto-optimal front compared to the Pareto-archived evolution strategy and the strength-Pareto evolutionary algorithm - two other elitist MOEAs that pay special attention to creating a diverse Pareto-optimal front. Moreover, we modify the definition of dominance in order to solve constrained multi-objective problems efficiently. Simulation results of the constrained NSGA-II on a number of test problems, including a five-objective, seven-constraint nonlinear problem, are compared with another constrained multi-objective optimizer, and the much better performance of NSGA-II is observed.
链接：https://ieeexplore.ieee.org/document/996017

25.标题：PiiGAN: Generative Adversarial Networks for Pluralistic Image Inpainting
出处：IEEE Access (Volume: 8)
作者：Weiwei Cai ; Zhanguo Wei
摘要：The latest methods based on deep learning have achieved amazing results regarding the complex work of inpainting large missing areas in an image. But this type of method generally attempts to generate one single “optimal” result, ignoring many other plausible results. Considering the uncertainty of the inpainting task, one sole result can hardly be regarded as a desired regeneration of the missing area. In view of this weakness, which is related to the design of the previous algorithms, we propose a novel deep generative model equipped with a brand new style extractor which can extract the style feature (latent vector) from the ground truth. Once obtained, the extracted style feature and the ground truth are both input into the generator. We also craft a consistency loss that guides the generated image to approximate the ground truth. After iterations, our generator is able to learn the mapping of styles corresponding to multiple sets of vectors. The proposed model can generate a large number of results consistent with the context semantics of the image. Moreover, we evaluated the effectiveness of our model on three datasets, i.e., CelebA, PlantVillage, and MauFlex. Compared to state-of-the-art inpainting methods, this model is able to offer desirable inpainting results with both better quality and higher diversity. The code and model will be made available on https://github.com/vivitsai/PiiGAN .
链接：https://ieeexplore.ieee.org/document/9027849

ESI HOT PAPERS

(Chemistry)

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

1、被引频次：605

题目：ORGANIC AND SOLUTION-PROCESSED TANDEM SOLAR CELLS WITH 17.3% EFFICIENCY

作者： MENG, LX;ZHANG, YM;WAN, XJ;LI, CX;ZHANG, X;WANG, YB;KE, X;XIAO, Z;DING, LM;XIA, RX;YIP, HL;CAO, Y;CHEN, YS

出处：SCIENCE 361 (6407): 1094-+ SEP 14 2018

摘要：Although organic photovoltaic (OPV) cells have many advantages, their performance still lags far behind that of other photovoltaic platforms. A fundamental reason for their low performance is the low charge mobility of organic materials, leading to a limit on the active-layer thickness and efficient light absorption. In this work, guided by a semi-empirical model analysis and using the tandem cell strategy to overcome such issues, and taking advantage of the high diversity and easily tunable band structure of organic materials, a record and certified 17.29% power conversion efficiency for a two-terminal monolithic solution-processed tandem OPV is achieved.

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2、被引频次：452

题目：SOFTWARE UPDATE: THE ORCA PROGRAM SYSTEM, VERSION 4.0

作者：NEESE, F

出处：WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE 8 (1): - JAN-FEB 2018

摘要：This short update provides an overview of the capabilities that have been added to the ORCA electronic structure package (version 4.0) since publication of the first article in 2012. (C) 2017 Wiley Periodicals, Inc.

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3、被引频次：437

题目：METAL-ORGANIC FRAMEWORK-BASED MATERIALS: SUPERIOR ADSORBENTS FOR THE CAPTURE OF TOXIC AND RADIOACTIVE METAL IONS

作者：LI, J;WANG, XX;ZHAO, GX;CHEN, CL;CHAI, ZF;ALSAEDI, A;HAYAT, T;WANG, XK

出处：CHEMICAL SOCIETY REVIEWS 47 (7): 2322-2356 APR 7 2018

摘要：Highly efficient removal of metal ion pollutants, such as toxic and nuclear waste-related metal ions, remains a serious task from the biological and environmental standpoint because of their harmful effects on human health and the environment. Recently, highly porous metal-organic frameworks (MOFs), with excellent chemical stability and abundant functional groups, have represented a new addition to the area of capturing various types of hazardous metal ion pollutants. This review focuses on recent progress in reported MOFs and MOF-based composites as superior adsorbents for the efficient removal of toxic and nuclear waste-related metal ions. Aspects related to the interaction mechanisms between metal ions and MOF-based materials are systematically summarized, including macroscopic batch experiments, microscopic spectroscopy analysis, and theoretical calculations. The adsorption properties of various MOF-based materials are assessed and compared with those of other widely used adsorbents. Finally, we propose our personal insights into future research opportunities and challenges in the hope of stimulating more researchers to engage in this new field of MOF-based materials for environmental pollution management.

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4、被引频次：345

题目：A WIDE BAND GAP POLYMER WITH A DEEP HIGHEST OCCUPIED MOLECULAR ORBITAL LEVEL ENABLES 14.2% EFFICIENCY IN POLYMER SOLAR CELLS

作者：LI, SS;YE, L;ZHAO, WC;YAN, HP;YANG, B;LIU, DL;LI, WN;ADE, H;HOU, JH

出处：JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 140 (23): 7159-7167 JUN 13 2018

摘要：To simultaneously achieve low photon energy loss (E-loss) and broad spectral response, the molecular design of the wide band gap (WBG) donor polymer with a deep HOMO level is of critical importance in fullerene-free polymer solar cells (PSCs). Herein, we developed a new benzodithiophene unit, i.e., DTBDT-EF, and conducted systematic investigations on a WBG DTBDT-EF-based donor polymer, namely, PDTB-EF-T. Due to the synergistic electron-withdrawing effect of the fluorine atom and ester group, PDTB-EFT exhibits a higher oxidation potential, i.e., a deeper HOMO level (ca. -5.5 eV) than most well-known donor polymers. Hence, a high open-circuit voltage of 0.90 V was obtained when paired with a fluorinated small molecule acceptor (IT-4F), corresponding to a low E-loss, of 0.62 eV. Furthermore, side-chain engineering demonstrated that

subtle side-chain modulation of the ester greatly influences the aggregation effects and molecular packing of polymer PDTB-EF-T. With the benefits of the stronger interchain pi-pi interaction, the improved ordering structure, and thus the highest hole mobility, the most symmetric charge transport and reduced recombination are achieved for the linear decyl-substituted PDTB-EF-T (P2)-based PSCs, leading to the highest short-circuit current density and fill factor (FF). Due to the high Flory-Huggins interaction parameter (chi), surface-directed phase separation occurs in the P2:IT-4F blend, which is supported by X-ray photoemission spectroscopy results and cross-sectional transmission electron microscope images. By taking advantage of the vertical phase distribution of the P2:IT4F blend, a high power conversion efficiency (PCE) of 14.2% with an outstanding FF of 0.76 was recorded for inverted devices. These results demonstrate the great potential of the DTBDT-EF unit for future organic photovoltaic applications.

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5、被引频次：332

题目：METAL CATALYSTS FOR HETEROGENEOUS CATALYSIS: FROM SINGLE ATOMS TO NANOCLUSTERS AND NANOPARTICLES

作者：LIU, LC;CORMA, A

出处：CHEMICAL REVIEWS 118 (10): 4981-5079 MAY 23 2018

摘要：Metal species with different size (single atoms, nanoclusters, and nanoparticles) show different catalytic behavior for various heterogeneous catalytic reactions. It has been shown in the literature that many factors including the particle size, shape, chemical composition, metal-support interaction, and metal-reactant/solvent interaction can have significant influences on the catalytic properties of metal catalysts. The recent developments of well-controlled synthesis methodologies and advanced characterization tools allow one to correlate the relationships at the molecular level. In this Review, the electronic and geometric structures of single atoms, nanoclusters, and nanoparticles will be discussed. Furthermore, we will summarize the catalytic applications of single atoms, nanoclusters, and nanoparticles for different types of reactions, including CO oxidation, selective oxidation, selective hydrogenation, organic reactions, electrocatalytic, and photocatalytic reactions. We will compare the results obtained from different systems and try to give a picture on how different types of metal species work in different reactions and give perspectives on the future directions toward better understanding of the catalytic behavior of different metal entities (single atoms, nanoclusters, and nanoparticles) in a unifying manner.

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6、被引频次：329

题目：NONFULLERENE ACCEPTOR MOLECULES FOR BULK HETEROJUNCTION ORGANIC SOLAR CELLS

作者：ZHANG, GY;ZHAO, JB;CHOW, PCY;JIANG, K;ZHANG, JQ;ZHU, ZL;ZHANG, J;HUANG, F;YAN, H

出处：CHEMICAL REVIEWS 118 (7): 3447-3507 APR 11 2018

摘要：The bulk-heterojunction blend of an electron donor and an electron acceptor material is the key component in a solution-processed organic photovoltaic device. In the past decades, a p-type conjugated polymer and an n-type fullerene derivative have been the most commonly used electron donor and electron acceptor, respectively. While most advances of the device performance come from the design of new polymer donors, fullerene derivatives have almost been exclusively used as electron acceptors in organic photovoltaics. Recently, nonfullerene acceptor materials, particularly small molecules and oligomers, have emerged as a promising alternative to replace fullerene derivatives. Compared to fullerenes, these new acceptors are generally synthesized from diversified, low-cost routes based on building block materials with extraordinary chemical, thermal, and photostability. The facile functionalization of these molecules affords excellent tunability to their optoelectronic and electrochemical properties. Within the past five years, there have been over 100 nonfullerene acceptor molecules synthesized, and the power conversion efficiency of nonfullerene organic solar cells has increased dramatically, from similar to 2% in 2012 to >13% in 2017. This review summarizes this progress, aiming to describe the molecular design strategy, to provide insight into the structure-property relationship, and to highlight the challenges the field is facing, with emphasis placed on most recent nonfullerene acceptors that demonstrated top-of-the-line photovoltaic performances. We also provide perspectives from a device point of view, wherein topics including ternary blend device, multijunction device, device stability, active layer morphology, and device physics are discussed.

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7、被引频次：280

题目：EMERGING TWO-DIMENSIONAL NANOMATERIALS FOR ELECTROCATALYSIS

作者：JIN, HY;GUO, CX;LIU, X;LIU, JL;VASILEFF, A;JIAO, Y;ZHENG, Y;QIAO, SZ

出处：CHEMICAL REVIEWS 118 (13): 6337-6408 SP. ISS. SI JUL 11 2018

摘要：Over the past few decades, the design and development of advanced electrocatalysts for efficient energy conversion technologies have been subjects of extensive study. With the discovery of graphene, two-dimensional (2D) nanomaterials have emerged as some of the most promising candidates for heterogeneous electrocatalysts due to their unique physical, chemical, and electronic

properties. Here, we review 2D-nanomaterial-based electrocatalysts for selected electrocatalytic processes. We first discuss the unique advances in 2D electrocatalysts based on different compositions and functions followed by specific design principles. Following this overview, we discuss various 2D electrocatalysts for electrocatalytic processes involved in the water cycle, carbon cycle, and nitrogen cycle from their fundamental conception to their functional application. We place a significant emphasis on different engineering strategies for 2D nanomaterials and the influence these strategies have on intrinsic material performance, such as electronic properties and adsorption energetics. Finally, we feature the opportunities and challenges ahead for 2D nanomaterials as efficient electrocatalysts. By considering theoretical calculations, surface characterization, and electrochemical tests, we describe the fundamental relationships between electronic structure, adsorption energy, and apparent activity for a wide variety of 2D electrocatalysts with the goal of providing a better understanding of these emerging nanomaterials at the atomic level.

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8、被引频次：273

题目：MAXIMIZING AND STABILIZING LUMINESCENCE FROM HALIDE PEROVSKITES WITH POTASSIUM PASSIVATION

作者：ABDI-JALEBI, M;ANDAJI-GARMAROUDI, Z;CACOVICH, S;STAVRAKAS, C;PHILIPPE, B;RICHTER, JM;ALSARI, M;BOOKER, EP;HUTTER, EM;PEARSON, AJ;LILLIU, S;SAVENIJE, TJ;RENSMO, H;DIVITINI, G;DUCATI, C;FRIEND, RH;STRANKS, SD

出处：NATURE 555 (7697): 497-+ MAR 22 2018

摘要：Metal halide perovskites are of great interest for various high-performance optoelectronic applications(1). The ability to tune the perovskite bandgap continuously by modifying the chemical composition opens up applications for perovskites as coloured emitters, in building-integrated photovoltaics, and as components of tandem photovoltaics to increase the power conversion efficiency(2-4). Nevertheless, performance is limited by non-radiative losses, with luminescence yields in state-of-the-art perovskite solar cells still far from 100 per cent under standard solar illumination conditions(5-7). Furthermore, in mixed halide perovskite systems designed for continuous bandgap tunability(2) (bandgaps of approximately 1.7 to 1.9 electronvolts), photoinduced ion segregation leads to bandgap instabilities(8,9). Here we demonstrate substantial mitigation of both non-radiative losses and photoinduced ion migration in perovskite films and interfaces by decorating the surfaces and grain boundaries with passivating potassium halide layers. We demonstrate external photoluminescence quantum yields of 66 per cent, which translate to internal yields that exceed 95 per cent. The high luminescence yields are achieved while maintaining high mobilities of more than 40 square centimetres per volt per second, providing the elusive combination of both high luminescence and excellent charge transport(10). When interfaced with electrodes in a solar cell device stack, the external luminescence yielda quantity that must be maximized to obtain high efficiencyremains as high as 15 per cent, indicating very clean interfaces. We also demonstrate the inhibition of transient photoinduced ion-migration processes across a wide range of mixed halide perovskite bandgaps in materials that exhibit bandgap instabilities when unpassivated. We validate these results in fully operating solar cells. Our work represents an important advance in the construction of tunable metal halide perovskite films and interfaces that can approach the efficiency

limits in tandem solar cells, coloured-light-emitting diodes and other optoelectronic applications.
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9、被引频次：272
题目：CORE-SHELL ZIF-8@ZIF-67-DERIVED COP NANOPARTICLE-EMBEDDED N-DOPED CARBON NANOTUBE HOLLOW POLYHEDRON FOR EFFICIENT OVERALL WATER SPLITTING
作者：PAN, Y;SUN, KA;LIU, SJ;CAO, X;WU, KL;CHEONG, WC;CHEN, Z;WANG, Y;LI, Y;LIU, YQ;WANG, DS;PENG, Q;CHEN, C;LI, YD
出处：JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 140 (7): 2610-2618 FEB 21 2018
摘要：The construction of highly active and stable non-noble metal electrocatalysts for hydrogen and oxygen evolution reactions is a major challenge for overall water splitting. Herein, we report a novel hybrid nanostructure with CoP nanopartides (NPs) embedded in a N-doped carbon nanotube hollow polyhedron (NCNHP) through a pyrolysis-oxidation-phosphidation strategy derived from core-shell ZIF-8@ZIF-67. Benefiting from the synergistic effects between highly active CoP NPs and NCNHP, the CoP/NCNHP hybrid exhibited outstanding bifunctional electrocatalytic performances. When the CoP/NCNHP was employed as both the anode and cathode for overall water splitting, a potential as low as 1.64 V was needed to achieve the current density of 10 rnA.cm(-2), and it still exhibited superior activity after continuously working for 36 h with nearly negligible decay in potential. Density functional theory calculations indicated that the electron transfer from NCNHP to CoP could increase the electronic states of the Co d-orbital around the Fermi level, which could increase the binding strength with H and therefore improve the electrocatalytic performance. The strong stability is attributed to high oxidation resistance of the CoP surface protected by the NCNHP.
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10、被引频次：262
题目：HETEROGENEOUS SINGLE-ATOM CATALYSIS
作者：WANG, AQ;LI, J;ZHANG, T
出处：NATURE REVIEWS CHEMISTRY 2 (6): 65-81 JUN 2018
摘要：Single-atom catalysis has arguably become the most active new frontier in heterogeneous catalysis. Aided by recent advances in practical synthetic methodologies, characterization techniques and computational modelling, we now have a large number of single-atom catalysts (SACs) that

exhibit distinctive performances for a wide variety of chemical reactions. This Perspective summarizes recent experimental and computational efforts aimed at understanding the bonding in SACs and how this relates to catalytic performance. The examples described here illustrate the utility of SACs in a broad scope of industrially important reactions and highlight the advantages these catalysts have over those presently used. SACs have well-defined active centres, such that unique opportunities exist for the rational design of new catalysts with high activities, selectivities and stabilities. Indeed, given a certain practical application, we can often design a suitable SAC; thus, the field has developed very rapidly and afforded promising catalyst leads. Moreover, the control we have over certain SAC structures paves the way for designing base metal catalysts with the activities of noble metal catalysts. It appears that we are entering a new era of heterogeneous catalysis in which we have control over well-dispersed single-atom active sites whose properties we can readily tune.

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11、被引频次：255

题目：RATIONAL DESIGN OF ELECTROCATALYSTS AND PHOTO(ELECTRO) CATALYSTS FOR NITROGEN REDUCTION TO AMMONIA (NH3) UNDER AMBIENT CONDITIONS

作者：GUO, CX;RAN, JR;VASILEFF, A;QIAO, SZ

出处：ENERGY & ENVIRONMENTAL SCIENCE 11 (1): 45-56 JAN 2018

摘要：As one of the most important chemicals and carbon-free energy carriers, ammonia (NH3) has a worldwide annual production of similar to 150 million tons, and is mainly produced by the traditional high-temperature and high-pressure Haber-Bosch process which consumes massive amounts of energy. Very recently, electrocatalytic and photo(electro) catalytic reduction of N-2 to NH3, which can be performed at ambient conditions using renewable energy, have received tremendous attention. The overall performance of these electrocatalytic and photo(electro) catalytic systems is largely dictated by their core components, catalysts. This perspective for the first time highlights the rational design of electrocatalysts and photo(electro) catalysts for N-2 reduction to NH3 under ambient conditions. Fundamental theory of catalytic reaction pathways for the N-2 reduction reaction and the corresponding material design principles are introduced first. Then, recently developed electrocatalysts and photo(electro) catalysts are summarized, with a special emphasis on the relationship between their physicochemical properties and NH3 production performance. Finally, the opportunities in this emerging research field, in particular, the strategy of combining experimental and theoretical techniques to design efficient and stable catalysts for NH3 production, are outlined.

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12、被引频次：252

题目：LUMINESCENT SENSORS BASED ON METAL-ORGANIC FRAMEWORKS

作者：ZHANG, YM;YUAN, S;DAY, G;WANG, X;YANG, XY;ZHOU, HC

出处：COORDINATION CHEMISTRY REVIEWS 354: 28-45 SP. ISS. SI JAN 1 2018

摘要：Metal-organic frameworks (MOFs) are a fascinating class of highly porous materials composed of metal ions/clusters and organic linkers, which promise great potential in numerous fields. Recently, the use of MOFs as luminescent sensors has been extensively explored due to their unique crystallinity, tunable porosity and structural diversity. In this review, we intend to highlight some of recent studies in this active research area and update the database of various luminescent MOF-based sensors on the basis of different sensing targets including ions, organic molecules, and gases, and temperature. (C) 2017 Published by Elsevier B.V.

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13、被引频次：244

题目：CHEMICALS FROM LIGNIN: AN INTERPLAY OF LIGNOCELLULOSE FRACTIONATION, DEPOLYMERISATION, AND UPGRADING

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出处：CHEMICAL SOCIETY REVIEWS 47 (3): 852-908 FEB 7 2018

摘要：In pursuit of more sustainable and competitive biorefineries, the effective valorisation of lignin is key. An alluring opportunity is the exploitation of lignin as a resource for chemicals. Three technological biorefinery aspects will determine the realisation of a successful lignin-to-chemicals valorisation chain, namely (i) lignocellulose fractionation, (ii) lignin depolymerisation, and (iii) upgrading towards targeted chemicals. This review provides a summary and perspective of the extensive research that has been devoted to each of these three interconnected biorefinery aspects, ranging from industrially well-established techniques to the latest cutting edge innovations. To navigate the reader through the overwhelming collection of literature on each topic, distinct strategies/topics were delineated and summarised in comprehensive overview figures. Upon closer inspection, conceptual principles arise that rationalise the success of certain methodologies, and more importantly, can guide future research to further expand the portfolio of promising technologies. When targeting chemicals, a key objective during the fractionation and depolymerisation stage is to minimise lignin condensation (i.e. formation of resistive carbon-carbon linkages). During fractionation, this can be achieved by either (i) preserving the (native) lignin structure or (ii) by tolerating depolymerisation of the lignin polymer but preventing condensation through chemical quenching or physical removal of reactive intermediates. The latter strategy is also commonly applied in the lignin depolymerisation stage, while an alternative approach is to augment the relative rate of depolymerisation vs. condensation by enhancing the reactivity of the lignin structure towards depolymerisation. Finally, because depolymerised lignins often consist of a complex mixture of various compounds, upgrading of the raw product mixture through convergent transformations embodies a promising approach to decrease the complexity. This particular upgrading approach is termed funneling, and includes both chemocatalytic and biological strategies.

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14、被引频次：243
题目：SUSTAINABLE CONVERSION OF CARBON DIOXIDE: AN INTEGRATED REVIEW OF CATALYSIS AND LIFE CYCLE ASSESSMENT
作者：ARTZ, J;MULLER, TE;THENERT, K;KLEINEKORTE, J;MEYS, R;STERNBERG, A;BARDOW, A;LEITNER, W
出处：CHEMICAL REVIEWS 118 (2): 434-504 SP. ISS. SI JAN 24 2018
摘要：CO2 conversion covers a wide range of possible application areas from fuels to bulk and commodity chemicals and even to specialty products with biological activity such as pharmaceuticals. In the present review, we discuss selected examples in these areas in a combined analysis of the state-of-the-art of synthetic methodologies and processes with their life cycle assessment. Thereby, we attempted to assess the potential to reduce the environmental footprint in these application fields relative to the current petrochemical value chain. This analysis and discussion differs significantly from a viewpoint on CO2 utilization as a measure for global CO2 mitigation. Whereas the latter focuses on reducing the end-of-pipe problem "CO2 emissions" from todays' industries, the approach taken here tries to identify opportunities by exploiting a novel feedstock that avoids the utilization of fossil resource in transition toward more sustainable future production. Thus, the motivation to develop CO2-based chemistry does not depend primarily on the absolute amount of CO2 emissions that can be remediated by a single technology. Rather, CO2-based chemistry is stimulated by the significance of the relative improvement in carbon balance and other critical factors defining the environmental impact of chemical production in all relevant sectors in accord with the principles of green chemistry.
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15、被引频次：233
题目：VISIBLE-LIGHT PHOTOCATALYSIS: DOES IT MAKE A DIFFERENCE IN ORGANIC SYNTHESIS?
作者：MARZO, L;PAGIRE, SK;REISER, O;KONIG, B
出处：ANGEWANDTE CHEMIE-INTERNATIONAL EDITION 57 (32): 10034-10072 AUG 6 2018
摘要：Visible-light photocatalysis has evolved over the last decade into a widely used method in organic synthesis. Photocatalytic variants have been reported for many important transformations, such as cross-coupling reactions, -amino functionalizations, cycloadditions, ATRA reactions, or fluorinations. To help chemists select photocatalytic methods for their synthesis, we compare in this Review classical and photocatalytic procedures for selected classes of reactions and highlight their advantages and limitations. In many cases, the photocatalytic reactions proceed under milder reaction conditions, typically at room temperature, and stoichiometric reagents are replaced by simple

oxidants or reductants, such as air, oxygen, or amines. Does visible-light photocatalysis make a difference in organic synthesis? The prospect of shuttling electrons back and forth to substrates and intermediates or to selectively transfer energy through a visible-light-absorbing photocatalyst holds the promise to improve current procedures in radical chemistry and to open up new avenues by accessing reactive species hitherto unknown, especially by merging photocatalysis with organo- or metal catalysis.

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16、被引频次：232

题目：FROM LITHIUM-ION TO SODIUM-ION BATTERIES: ADVANTAGES, CHALLENGES, AND SURPRISES

作者：NAYAK, PK;YANG, LT;BREHM, W;ADELHELM, P

出处：ANGEWANDTE CHEMIE-INTERNATIONAL EDITION 57 (1): 102-120 JAN 2 2018

摘要：Mobile and stationary energy storage by rechargeable batteries is a topic of broad societal and economical relevance. Lithium-ion battery (LIB) technology is at the forefront of the development, but a massively growing market will likely put severe pressure on resources and supply chains. Recently, sodium-ion batteries (SIBs) have been reconsidered with the aim of providing a lower-cost alternative that is less susceptible to resource and supply risks. On paper, the replacement of lithium by sodium in a battery seems straightforward at first, but unpredictable surprises are often found in practice. What happens when replacing lithium by sodium in electrode reactions? This review provides a state-of-the art overview on the redox behavior of materials when used as electrodes in lithium-ion and sodium-ion batteries, respectively. Advantages and challenges related to the use of sodium instead of lithium are discussed.

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17、被引频次：232

题目：BRIGHT SIDE OF LIGNIN DEPOLYMERIZATION: TOWARD NEW PLATFORM CHEMICALS

作者：SUN, ZH;FRIDRICH, B;DE SANTI, A;ELANGOVAN, S;BARTA, K

出处：CHEMICAL REVIEWS 118 (2): 614-678 SP. ISS. SI JAN 24 2018

摘要：Lignin, a major component of lignocellulose, is the largest source of aromatic building blocks on the planet and harbors great potential to serve as starting material for the production of biobased products. Despite the initial challenges associated with the robust and irregular structure of lignin, the valorization of this intriguing aromatic biopolymer has come a long way: recently, many creative strategies emerged that deliver defined products via catalytic or biocatalytic depolymerization in good yields. The purpose of this review is to provide insight into these novel approaches and the potential application of such emerging new structures for the synthesis of biobased polymers or pharmacologically active molecules. Existing strategies for functionalization or defunctionalization

of lignin-based compounds are also summarized. Following the whole value chain from raw lignocellulose through depolymerization to application whenever possible, specific lignin-based compounds emerge that could be in the future considered as potential lignin-derived platform chemicals.

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18、被引频次：225

题目：TOWARDS FLEXIBLE SOLID-STATE SUPERCAPACITORS FOR SMART AND WEARABLE ELECTRONICS

作者：DUBAL, DP;CHODANKAR, NR;KIM, DH;GOMEZ-ROMERO, P

出处：CHEMICAL SOCIETY REVIEWS 47 (6): 2065-2129 MAR 21 2018

摘要：Flexible solid-state supercapacitors (FSSCs) are frontrunners in energy storage device technology and have attracted extensive attention owing to recent significant breakthroughs in modern wearable electronics. In this study, we review the state-of-the-art advancements in FSSCs to provide new insights on mechanisms, emerging electrode materials, flexible gel electrolytes and novel cell designs. The review begins with a brief introduction on the fundamental understanding of charge storage mechanisms based on the structural properties of electrode materials. The next sections briefly summarise the latest progress in flexible electrodes (i.e., freestanding and substrate-supported, including textile, paper, metal foil/wire and polymer-based substrates) and flexible gel electrolytes (i.e., aqueous, organic, ionic liquids and redox-active gels). Subsequently, a comprehensive summary of FSSC cell designs introduces some emerging electrode materials, including MXenes, metal nitrides, metal-organic frameworks (MOFs), polyoxometalates (POMs) and black phosphorus. Some potential practical applications, such as the development of piezoelectric, photo-, shape-memory, self-healing, electrochromic and integrated sensor-supercapacitors are also discussed. The final section highlights current challenges and future perspectives on research in this thriving field.

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19、被引频次：221

题目：ROLE OF BIOCATALYSIS IN SUSTAINABLE CHEMISTRY

作者：SHELDON, RA;WOODLEY, JM

出处：CHEMICAL REVIEWS 118 (2): 801-838 SP. ISS. SI JAN 24 2018

摘要：Based on the principles and metrics of green chemistry and sustainable development, biocatalysis is both a green and sustainable technology. This is largely a result of the spectacular advances in molecular biology and biotechnology achieved in the past two decades. Protein engineering has enabled the optimization of existing enzymes and the invention of entirely new biocatalytic reactions that were previously unknown in Nature. It is now eminently feasible to

develop enzymatic transformations to fit predefined parameters, resulting in processes that are truly sustainable by design. This approach has successfully been applied, for example, in the industrial synthesis of active pharmaceutical ingredients. In addition to the use of protein engineering, other aspects of biocatalysis engineering, such as substrate, medium, and reactor engineering, can be utilized to improve the efficiency and cost-effectiveness and, hence, the sustainability of biocatalytic reactions. Furthermore, immobilization of an enzyme can improve its stability and enable its reuse multiple times, resulting in better performance and commercial viability. Consequently, biocatalysis is being widely applied in the production of pharmaceuticals and some commodity chemicals. Moreover, its broader application will be further stimulated in the future by the emerging biobased economy.

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20、被引频次：219

题目：USE OF ELECTROCHEMISTRY IN THE SYNTHESIS OF HETEROCYCLIC STRUCTURES

作者：JIANG, YY;XU, K;ZENG, CC

出处：CHEMICAL REVIEWS 118 (9): 4485-4540 SP. ISS. SI MAY 9 2018

摘要：The preparation and transformation of heterocyclic structures have always been of great interest in organic chemistry. Electrochemical technique provides a versatile and powerful approach to the assembly of various heterocyclic structures. In this review, we examine the advance in relation to the electrochemical construction of heterocyclic compounds published since 2000 via intra- and intermolecular cyclization reactions.

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21、被引频次：216

题目：GENERAL SYNTHESIS AND DEFINITIVE STRUCTURAL IDENTIFICATION OF MN4C4 SINGLE-ATOM CATALYSTS WITH TUNABLE ELECTROCATALYTIC ACTIVITIES

作者：FEI, HL;DONG, JC;FENG, YX;ALLEN, CS;WAN, CZ;VOLOSSKIY, B;LI, MF;ZHAO, ZP;WANG, YL;SUN, HT;AN, PF;CHEN, WX;GUO, ZY;LEE, C;CHEN, DL;SHAKIR, I;LIU, MJ;HU, TD;LI, YD;KIRKLAND, AI;DUAN, XF;HUANG, Y

出处：NATURE CATALYSIS 1 (1): 63-72 JAN 2018

摘要：Single-atom catalysts (SACs) have recently attracted broad research interest as they combine the merits of both homogeneous and heterogeneous catalysts. Rational design and synthesis of SACs are of immense significance but have so far been plagued by the lack of a definitive correlation between structure and catalytic properties. Here, we report a general approach to a series of monodispersed atomic transition metals (for example, Fe, Co, Ni) embedded in nitrogen-doped

graphene with a common MN4C4 moiety, identified by systematic X-ray absorption fine structure analyses and direct transmission electron microscopy imaging. The unambiguous structure determination allows density functional theoretical prediction of MN4C4 moieties as efficient oxygen evolution catalysts with activities following the trend Ni > Co > Fe, which is confirmed by electrochemical measurements. Determination of atomistic structure and its correlation with catalytic properties represents a critical step towards the rational design and synthesis of precious or nonprecious SACs with exceptional atom utilization efficiency and catalytic activities.

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22、被引频次：211

题目：CO2 ELECTROREDUCTION TO ETHYLENE VIA HYDROXIDE-MEDIATED COPPER CATALYSIS AT AN ABRUPT INTERFACE

作 者：DINH, CT;BURDYNY, T;KIBRIA, MG;SEIFITOKALDANI, A;GABARDO, CM;DE ARQUER, FPG;KIANI, A;EDWARDS, JP;DE LUNA, P;BUSHUYEV, OS;ZOU, CQ;QUINTERO-BERMUDEZ, R;PANG, YJ;SINTON, D;SARGENT, EH

出处：SCIENCE 360 (6390): 783-787 SP. ISS. SI MAY 18 2018

摘要：Carbon dioxide (CO2) electroreduction could provide a useful source of ethylene, but low conversion efficiency, low production rates, and low catalyst stability limit current systems. Here we report that a copper electrocatalyst at an abrupt reaction interface in an alkaline electrolyte reduces CO2 to ethylene with 70% faradaic efficiency at a potential of -0.55 volts versus a reversible hydrogen electrode (RHE). Hydroxide ions on or near the copper surface lower the CO2 reduction and carbon monoxide (CO)-CO coupling activation energy barriers; as a result, onset of ethylene evolution at -0.165 volts versus an RHE in 10 molar potassium hydroxide occurs almost simultaneously with CO production. Operational stability was enhanced via the introduction of a polymer-based gas diffusion layer that sandwiches the reaction interface between separate hydrophobic and conductive supports, providing constant ethylene selectivity for an initial 150 operating hours.

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23、被引频次：206

题目：RECENT PROGRESS IN 2D GROUP-VA SEMICONDUCTORS: FROM THEORY TO EXPERIMENT

作者：ZHANG, SL;GUO, SY;CHEN, ZF;WANG, YL;GAO, HJ;GOMEZ-HERRERO, J;ARES, P;ZAMORA, F;ZHU, Z;ZENG, HB

出处：CHEMICAL SOCIETY REVIEWS 47 (3): 982-1021 FEB 7 2018

摘要：Phosphorene, an emerging two-dimensional material, has received considerable attention due to its layer-controlled direct bandgap, high carrier mobility, negative Poisson's ratio and unique in-plane anisotropy. As cousins of phosphorene, 2D group-VA arsenene, antimonene and bismuthene have also garnered tremendous interest due to their intriguing structures and fascinating electronic properties. 2D group-VA family members are opening up brand-new opportunities for their multifunctional applications encompassing electronics, optoelectronics, topological spintronics, thermoelectrics, sensors, Li-or Na-batteries. In this review, we extensively explore the latest theoretical and experimental progress made in the fundamental properties, fabrications and applications of 2D group-VA materials, and offer perspectives and challenges for the future of this emerging field.

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24、被引频次：204

题目：MAGNETIC HYSTERESIS UP TO 80 KELVIN IN A DYSPROSIUM METALLOCENE SINGLE-MOLECULE MAGNET

作者：GUO, FS;DAY, BM;CHEN, YC;TONG, ML;MANSIKKAMAKI, A;LAYFIELD, RA

出处：SCIENCE 362 (6421): 1400-+ SP. ISS. SI DEC 21 2018

摘要：Single-molecule magnets (SMMs) containing only one metal center may represent the lower size limit for molecule-based magnetic information storage materials. Their current drawback is that all SMMs require liquid-helium cooling to show magnetic memory effects. We now report a chemical strategy to access the dysprosium metallocene cation [(Cp-iPr5)Dy(Cp*)](+) (Cp-iPr5, penta-iso-propylcyclopentadienyl; Cp*, pentamethylcyclopentadienyl), which displays magnetic hysteresis above liquid-nitrogen temperatures. An effective energy barrier to reversal of the magnetization of U-eff = 1541 wave number is also measured. The magnetic blocking temperature of T-B = 80 kelvin for this cation overcomes an essential barrier toward the development of nanomagnet devices that function at practical temperatures.

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25、被引频次：203
题目：CARBON CAPTURE AND STORAGE (CCS): THE WAY FORWARD
作者：BUI, M;ADJIMAN, CS;BARDOW, A;ANTHONY, EJ;BOSTON, A;BROWN, S;FENNELL, PS;FUSS, S;GALINDO, A;HACKETT, LA;HALLETT, JP;HERZOG, HJ;JACKSON, G;KEMPER, J;KREVOR, S;MAITLAND, GC;MATUSZEWSKI, M;METCALFE, IS;PETIT, C;PUXTY, G;REIMER, J;REINER, DM;RUBIN, ES;SCOTT, SA;SHAH, N;SMIT, B;TRUSLER, JPM;WEBLEY, P;WILCOX, J;MAC DOWELL, N
出处：ENERGY & ENVIRONMENTAL SCIENCE 11 (5): 1062-1176 MAY 1 2018
摘要：Carbon capture and storage (CCS) is broadly recognised as having the potential to play a key role in meeting climate change targets, delivering low carbon heat and power, decarbonising industry and, more recently, its ability to facilitate the net removal of CO2 from the atmosphere. However, despite this broad consensus and its technical maturity, CCS has not yet been deployed on a scale commensurate with the ambitions articulated a decade ago. Thus, in this paper we review the current state-of-the-art of CO2 capture, transport, utilisation and storage from a multi-scale perspective, moving from the global to molecular scales. In light of the COP21 commitments to limit warming to less than 2 degrees C, we extend the remit of this study to include the key negative emissions technologies (NETs) of bioenergy with CCS (BECCS), and direct air capture (DAC). Cognisant of the non-technical barriers to deploying CCS, we reflect on recent experience from the UK's CCS commercialisation programme and consider the commercial and political barriers to the large-scale deployment of CCS. In all areas, we focus on identifying and clearly articulating the key research challenges that could usefully be addressed in the coming decade.
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ESI HIGHLY CITED PAPERS

(Chemistry)

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

1、被引频次：11789
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：JOURNAL OF CHEMICAL PHYSICS 132 (15): - APR 21 2010
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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2、被引频次：11725
题目：CRYSTAL STRUCTURE REFINEMENT WITH SHELXL
作者：SHELDRICK, GM
出处：ACTA CRYSTALLOGRAPHICA SECTION C-STRUCTURAL CHEMISTRY 71: 3-8 PART

1 JAN 2015

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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3、被引频次：7612

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

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

出处：JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 131 (17): 6050-+ MAY 6 2009

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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4、被引频次：6759

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：JOURNAL OF COMPUTATIONAL CHEMISTRY 31 (2): 455-461 JAN 30 2010

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

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5、被引频次：6460

题目：THE CHEMISTRY OF GRAPHENE OXIDE

作者：DREYER, DR;PARK, S;BIELAWSKI, CW;RUOFF, RS

出处：CHEMICAL SOCIETY REVIEWS 39 (1): 228-240 2010

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).

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6、被引频次：6254

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：JOURNAL OF COMPUTATIONAL CHEMISTRY 30 (16): 2785-2791 DEC 30 2009

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

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7、被引频次：5841

题目：DYE-SENSITIZED SOLAR CELLS

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

出处：CHEMICAL REVIEWS 110 (11): 6595-6663 NOV 2010

摘要：

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8、被引频次：5764
题目：HETEROGENEOUS PHOTOCATALYST MATERIALS FOR WATER SPLITTING
作者：KUDO, A;MISEKI, Y
出处：CHEMICAL SOCIETY REVIEWS 38 (1): 253-278 2009
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).
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9、被引频次：5613
题目：VESTA 3 FOR THREE-DIMENSIONAL VISUALIZATION OF CRYSTAL, VOLUMETRIC AND MORPHOLOGY DATA
作者：MOMMA, K;IZUMI, F
出处：JOURNAL OF APPLIED CRYSTALLOGRAPHY 44: 1272-1276 PART 6 DEC 2011
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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10、被引频次：5475

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

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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11、被引频次：5431

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

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.
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12、被引频次：5308
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
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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13、被引频次：5219
题目：SOLAR WATER SPLITTING CELLS
作 者：WALTER, MG;WARREN, EL;MCKONE, JR;BOETTCHER, SW;MI, QX;SANTORI, EA;LEWIS, NS
出处：CHEMICAL REVIEWS 110 (11): 6446-6473 NOV 2010
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14、被引频次：5128
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：JOURNAL OF PHYSICAL CHEMISTRY B 113 (18): 6378-6396 MAY 7 2009
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.

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15、被引频次：5068
题目：METAL-ORGANIC FRAMEWORK MATERIALS AS CATALYSTS
作者：LEE, J;FARHA, OK;ROBERTS, J;SCHEIDT, KA;NGUYEN, ST;HUPP, JT
出处：CHEMICAL SOCIETY REVIEWS 38 (5): 1450-1459 2009
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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16、被引频次：4983
题目：SELECTIVE GAS ADSORPTION AND SEPARATION IN METAL-ORGANIC FRAMEWORKS
作者：LI, JR;KUPPLER, RJ;ZHOU, HC
出处：CHEMICAL SOCIETY REVIEWS 38 (5): 1477-1504 2009
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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17、被引频次：4954
题目：EFFECT OF THE DAMPING FUNCTION IN DISPERSION CORRECTED DENSITY FUNCTIONAL THEORY
作者：GRIMME, S;EHRLICH, S;GOERIGK, L
出处：JOURNAL OF COMPUTATIONAL CHEMISTRY 32 (7): 1456-1465 MAY 2011
摘要：It is shown by an extensive benchmark on molecular energy data that the mathematical form of the damping function in DFT-D methods has only a minor impact on the quality of the results. For 12 different functionals, a standard "zero-damping" formula and rational damping to finite values for small interatomic distances according to Becke and Johnson (BJ-damping) has been tested. The same (DFT-D3) scheme for the computation of the dispersion coefficients is used. The BJ-damping requires one fit parameter more for each functional (three instead of two) but has the advantage of avoiding repulsive interatomic forces at shorter distances. With BJ-damping better results for nonbonded distances and more clear effects of intramolecular dispersion in four representative molecular structures are found. For the noncovalently-bonded structures in the S22 set, both schemes lead to very similar intermolecular distances. For noncovalent interaction energies BJ-damping

performs slightly better but both variants can be recommended in general. The exception to this is Hartree-Fock that can be recommended only in the BJ-variant and which is then close to the accuracy of corrected GGAs for non-covalent interactions. According to the thermodynamic benchmarks BJ-damping is more accurate especially for medium-range electron correlation problems and only small and practically insignificant double-counting effects are observed. It seems to provide a physically correct short-range behavior of correlation/dispersion even with unmodified standard functionals. In any case, the differences between the two methods are much smaller than the overall dispersion effect and often also smaller than the influence of the underlying density functional. (C) 2011 Wiley Periodicals, Inc. J Comput Chem 32: 1456-1465, 2011

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18、被引频次：4892

题目：THE CHEMISTRY AND APPLICATIONS OF METAL-ORGANIC FRAMEWORKS

作者：FURUKAWA, H;CORDOVA, KE;OKEEFFE, M;YAGHI, OM

出处：SCIENCE 341 (6149): 974-+ AUG 30 2013

摘要：Crystalline metal-organic frameworks (MOFs) are formed by reticular synthesis, which creates strong bonds between inorganic and organic units. Careful selection of MOF constituents can yield crystals of ultrahigh porosity and high thermal and chemical stability. These characteristics allow the interior of MOFs to be chemically altered for use in gas separation, gas storage, and catalysis, among other applications. The precision commonly exercised in their chemical modification and the ability to expand their metrics without changing the underlying topology have not been achieved with other solids. MOFs whose chemical composition and shape of building units can be multiply varied within a particular structure already exist and may lead to materials that offer a synergistic combination of properties.

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19、被引频次：4758

题目：A REVIEW OF ELECTRODE MATERIALS FOR ELECTROCHEMICAL SUPERCAPACITORS

作者：WANG, GP;ZHANG, L;ZHANG, JJ

出处：CHEMICAL SOCIETY REVIEWS 41 (2): 797-828 2012

摘要：In this critical review, metal oxides-based materials for electrochemical supercapacitor (ES) electrodes are reviewed in detail together with a brief review of carbon materials and conducting polymers. Their advantages, disadvantages, and performance in ES electrodes are discussed through extensive analysis of the literature, and new trends in material development are also reviewed. Two important future research directions are indicated and summarized, based on results published in the

literature: the development of composite and nanostructured ES materials to overcome the major challenge posed by the low energy density of ES (476 references).

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20、被引频次：4526

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

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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21、被引频次：4507

题目：MULTIWFN: A MULTIFUNCTIONAL WAVEFUNCTION ANALYZER

作者：LU, T;CHEN, FW

出处：JOURNAL OF COMPUTATIONAL CHEMISTRY 33 (5): 580-592 FEB 15 2012

摘要：Multiwfn is a multifunctional program for wavefunction analysis. Its main functions are: (1) Calculating and visualizing real space function, such as electrostatic potential and electron localization function at point, in a line, in a plane or in a spatial scope. (2) Population analysis. (3) Bond order analysis. (4) Orbital composition analysis. (5) Plot density-of-states and spectrum. (6) Topology analysis for electron density. Some other useful utilities involved in quantum chemistry studies are also provided. The built-in graph module enables the results of wavefunction analysis to be plotted directly or exported to high-quality graphic file. The program interface is very user-friendly and suitable for both research and teaching purpose. The code of Multiwfn is

substantially optimized and parallelized. Its efficiency is demonstrated to be significantly higher than related programs with the same functions. Five practical examples involving a wide variety of systems and analysis methods are given to illustrate the usefulness of Multiwfn. The program is free of charge and open-source. Its precompiled file and source codes are available from . (c) 2011 Wiley Periodicals, Inc. J Comput Chem, 2011

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22、被引频次：4433

题目：SEMICONDUCTOR-BASED PHOTOCATALYTIC HYDROGEN GENERATION

作者：CHEN, XB;SHEN, SH;GUO, LJ;MAO, SS

出处：CHEMICAL REVIEWS 110 (11): 6503-6570 NOV 2010

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23、被引频次：4290

题目：THE CHEMISTRY OF TWO-DIMENSIONAL LAYERED TRANSITION METAL DICHALCOGENIDE NANOSHEETS

作者：CHHOWALLA, M;SHIN, HS;EDA, G;LI, LJ;LOH, KP;ZHANG, H

出处：NATURE CHEMISTRY 5 (4): 263-275 APR 2013

摘要：Ultrathin two-dimensional nanosheets of layered transition metal dichalcogenides (TMDs) are fundamentally and technologically intriguing. In contrast to the graphene sheet, they are chemically versatile. Mono-or few-layered TMDs - obtained either through exfoliation of bulk materials or bottom-up syntheses - are direct-gap semiconductors whose bandgap energy, as well as carrier type (n- or p-type), varies between compounds depending on their composition, structure and dimensionality. In this Review, we describe how the tunable electronic structure of TMDs makes them attractive for a variety of applications. They have been investigated as chemically active electrocatalysts for hydrogen evolution and hydrosulfurization, as well as electrically active materials in opto-electronics. Their morphologies and properties are also useful for energy storage applications such as electrodes for Li-ion batteries and supercapacitors.

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24、被引频次：4274

题 目 ： NITROGEN-DOPED CARBON NANOTUBE ARRAYS WITH HIGH ELECTROCATALYTIC ACTIVITY FOR OXYGEN REDUCTION

作者：GONG, KP;DU, F;XIA, ZH;DURSTOCK, M;DAI, LM

出处：SCIENCE 323 (5915): 760-764 FEB 6 2009

摘要：The large- scale practical application of fuel cells will be difficult to realize if the expensive platinum- based electrocatalysts for oxygen reduction reactions (ORRs) cannot be replaced by other efficient, low- cost, and stable electrodes. Here, we report that vertically aligned nitrogen- containing carbon nanotubes (VA- NCNTs) can act as a metal- free electrode with a much better electrocatalytic activity, long- term operation stability, and tolerance to crossover effect than platinum for oxygen reduction in alkaline fuel cells. In air- saturated 0.1 molar potassium hydroxide, we observed a steady- state output potential of - 80 millivolts and a current density of 4.1 milliamps per square centimeter at - 0.22 volts, compared with - 85 millivolts and 1.1 milliamps per square centimeter at - 0.20 volts for a platinum- carbon electrode. The incorporation of electron- accepting nitrogen atoms in the conjugated nanotube carbon plane appears to impart a relatively high positive charge density on adjacent carbon atoms. This effect, coupled with aligning the NCNTs, provides a four- electron pathway for the ORR on VA- NCNTs with a superb performance.

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25、被引频次：4238

题 目 ： PALLADIUM-CATALYZED LIGAND-DIRECTED C-H FUNCTIONALIZATION REACTIONS

作者：LYONS, TW;SANFORD, MS

出处：CHEMICAL REVIEWS 110 (2): 1147-1169 FEB 2010

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AIAA、AAS 最新会议

AIAA

（AIAA 来源：http://www.aiaa.org/）

1.**会议名称：**2020 Integrated Communications Navigation and Surveillance Conference (ICNS)
会议时间：9 September - 11 September 2020
会议地点：Westin Washington Dulles Airport, Herndon, Virginia
会议简介：The Integrated Communications Navigation and Surveillance (ICNS) Conference, originally scheduled for 21–23 April 2020, is now scheduled for 9–11 September 2020. ICNS is the premier international aviation conference addressing technology and policy advances in CNS research, development and implementation programs, and policies related to CNS/ATM capabilities and applications. The ICNS Conference assembles leaders from government, industry, and academia, as well as senior technical experts to address important policy issues and contribute to the future directions of CNS and ATM.
链接：
https://www.aiaa.org/events-learning/event/2020/09/09/default-calendar/2020-integrated-communications-navigation-and-surveillance-conference-(icns)

2.**会议名称：**32nd Congress of the International Council of the Aeronautical Sciences (ICAS)
会议时间：14 September - 18 September 2020
会议地点：Shanghai, China
会议简介：ICAS is an international, non-government, non-profit scientific organization with the mission to advance knowledge and facilitate collaboration in aeronautics. ICAS is the only international support organization to representative aeronautical engineering professional societies and their members in 30 countries. ICAS organizes every two years an International Congress covering all aspects of aeronautical science and technology and their application to both military and civil aviation.
链接：
https://www.aiaa.org/events-learning/event/2020/09/14/default-calendar/32nd-congress-of-the-international-council-of-the-aeronautical-sciences-(icas)

3.**会议名称：**39th Digital Avionics Systems Conference (DASC)
会议时间：11 October - 15 October 2020
会议地点：Wyndham San Antonio River Walk, San Antonio, Texas
会议简介：Please join us in San Antonio, Texas for the 39th AIAA/IEEE Digital Avionics Systems Conference (DASC), the preeminent R&D Conference in the field of digital avionics offered by its two most distinguished professional societies, the Digital Avionics Technical Committee (DATC) of the American Institute of Aeronautics and Astronautics (AIAA) and the Aerospace and Electronic

Systems Society (AESS) of the Institute of Electrical and Electronics Engineers (IEEE).

In addition to its rich history, San Antonio offers plenty of educational, cultural and recreational opportunities for everyone to explore around the conference. Venture out to all of San Antonio's wonderful attractions including its world famous River Walk. We are positive that you will have a memorable and educational experience at the 39th DASC.

链接：

https://www.aiaa.org/events-learning/event/2020/10/11/default-calendar/39th-digital-avionics-systems-conference-(dasc)

4.**会议名称：**ASCEND – Accelerating Space Commerce Exploration and New Discovery

会议时间：16 NOVEMBER - 18 NOVEMBER 2020

会议地点：Las Vegas, Nevada, USA

会议简介：ASCEND is operating as scheduled, at this time. We encourage everyone to follow the coronavirus safety guidelines set out by the WHO and CDC. Updates about AIAA forums and events affected by the coronavirus response can be found here: www.aiaa.org/coronavirus

As we embark on a bold new era of space exploration, AIAA's ASCEND provides you with something few space events can: a seat at the table.

The new space economy is ready for takeoff. In the coming years, it's anticipated to skyrocket from $4 billion today to more than $1 trillion. This phenomenal growth will be driven by a number of factors, but none more important than you.

链接：

https://www.aiaa.org/events-learning/event/2020/11/16/default-calendar/ascend

5.**会议名称：**43rd Scientific Assembly of the Committee on Space Research (COSPAR) and Associated Events (Rescheduled)

会议时间：28 January - 4 February 2021

会议地点：Sydney, Australia

会议简介：The 43rd Scientific Assembly of the Committee on Space Research and Associated Events (COSPAR 2020), originally set for 15–22 August 2020, has been rescheduled for 28 January–4 February 2021.

The 2021 Assembly will combine the latest in space research findings with activities designed to enrich the global space research community - including helping equip our future leaders, and workshopping with space industry - and inspire the next generation of scientists and engineers. You will have the opportunity of a lifetime to interact directly with everything that Australia has to offer – our science and innovation, our people, our heritage, and our beautiful environment.

链接：

https://www.aiaa.org/events-learning/event/2021/01/28/default-calendar/43rd-scientific-assembly-of-the-committee-on-space-research-(cospar)-and-associated-events-(cospar-2020)

AAS

（AAS 来源：http://astronautical.org/）

1.**会议名称：**Wernher von Braun Memorial Symposium
会议时间：October 26-28, 2020
会议地点：Huntsville, Alabama
会议简介：The Wernher von Braun Memorial Symposium is an annual event that features panel discussions and guest speakers reflecting government, industry, academia, business and international perspectives on space exploration.
链接：https://astronautical.org/events/vonbraun/

ACM 最新会议

来源：http://www.acm.org/

1. **会议名称：**ACM BCB
会议时间：Aug 30-Sep2, 2020
会议地点：“virtual” mode
会议简介：UPDATE (as of April 1, 2020):
We have been closely monitoring the evolving situation with COVID-19 and its impact on various events. In the interest of ensuring health and safety for all attendees, and in anticipation of any continued travel restrictions extending later into the year and the uncertainties that may create, we have decided to move the ACM-BCB 2020 into a completely “virtual” mode. The precise format and platform details are being worked out and we will post those details as and when they become available. The conference and associated events will still happen around the designated dates albeit in a virtual mode. All calls (for papers, workshops, tutorials, highlights, posters) are on and will proceed as per original plan. Please refer to those individual links on this webpage for more details. We thank you for your interest in ACM-BCB.
-ACM-BCB 2020 Organizing Team
The 11th ACM Conference on Bioinformatics, Computational Biology, and Health Informatics (ACM BCB) is the flagship conference of the ACM SIGBio. ACM-BCB 2020 is the conference's eleventh year, building upon the success of the first ten meetings in Boston, Niagara Falls, Chicago, Orlando, Washington DC, Newport Beach, Atlanta, Seattle, Washington DC, and Niagara Falls. ACM-BCB 2020 will be held as a virtual conference due to COVID-19.
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.
链接：http://acm-bcb.org/2020/

2.**会议名称：**SETN 2020
会议时间：2-4 of September, 2020
会议地点：Athens, Greece
会议简介：The 11th Hellenic Conference on Artificial Intelligence (SETN 2020) will be held in Athens, Greece 2-4 of September, 2020. SETN conferences are organized biannually by the Hellenic Artificial Intelligence Society (EETN). SETN has already been established as one of the most prominent forums for Greek and International AI scientists to present original and high-quality research on emergent topics of Artificial Intelligence. The official language of the conferences is English.

SETN 2020 is organized by the Hellenic Artificial Intelligence Society (EETN) in collaboration with the Institute of Informatics and Telecommunications of NCSR "Demokritos", the Department of Informatics of the Athens University of Economics and Business, the Department of Informatics and Telematics of the Harokopio University of Athens and the Department of Informatics and Computer Engineering of the University of West Attica.

SETN 2020 highly encourages international participation. Note that SETN 2020 apart from the Research Track it accommodates an Industry Track as well.

Research Track intends for papers presenting unpublished, substantial, novel research and technology in ANY area of AI either Theoretical or Applied one.

Industry Track intends for presentations by professionals of real-life operational or near-to-market systems in which AI plays an important role. Emphasis should be given on how AI solves real-life needs.

链接：http://www.eetn.gr/setn2020/index.php/setn-2020-organisation/setn-2020-conference

3.**会议名称：**ICIBE 2020

会议时间：September 27-29, 2020

会议地点：Macau, China

会议简介：Conference Flyer

Due to the outbreak of the coronavirus, Online/Video Presentation are acceptable on the conference. Online presentation session will be arranged accordingly. Please contact the conference secretary for more information about Online/Video Presentation. Participants are required to wear face mask when attending the conference. And conference staff will check the body temperature and take other active action.

Welcome to the official website of the 2020 The 6th International Conference on Industrial and Business Engineering (ICIBE 2020), which will be held during September 27-29, 2020 in Macau, China.

ICIBE 2020 aims to bring together researchers, scientists, engineers, and scholar students to exchange and share their experiences, new ideas, and research results about all aspects of Industrial and Business Engineering, and discuss the practical challenges encountered and the solutions adopted. The conference will be held every year to make it an ideal platform for people to share views and experiences in Industrial and Business Engineering and related areas. For more details of the conference schedule, please feel free to contact us at icibe@iedrc.net. The full version of program will be given in October.

Notes: If the conference cannot be held on time due to the force majeure such as politics, weather and disasters, the organizer shall have the right to postpone or cancel the conference. Participants are required to comply with the organizer's arrangements and refund policy.

链接：http://www.icibe.org/

4.**会议名称：**SIGDOC Conference 2020

会议时间：3-4 Oct. 2020

会议地点：Denton, TX

会议简介：We are writing to inform you that as of right now SIGDOC 2020 in Denton, TX is still scheduled to be held as planned (October 3-4, 2020). Even though we are seven months out from the

event, we want to be transparent and active in our communication with you. The safety and well-being of all conference participants is of course our priority, and as such we are—as everyone is—following updates on the situation from the World Health Organization (WHO) and the Center for Disease Control (CDC).

链接：https://sigdoc.acm.org/conference/2020/#page-content

5.**会议名称：**IoT 2020

会议时间：Oct 6 - 9, 2020

会议地点：Malmö, Sweden

会议简介：The 10th International Conference on the Internet of Things (IoT 2020), building on the success of its predecessors since 2008, is the premier forum to share, discuss and witness cutting edge research in all areas of development for the Internet of Things.

The Internet of Things Conference is seeking original, high impact research papers on all topics related to the development of the Internet of Things. Papers will be reviewed and selected based on technical novelty, integrity of the analysis and social-environmental impacts and practical relevance.

In addition to the main conference track, there will be a Doctoral Colloquium and a workshop program.

链接：https://iot-conference.org/iot2020/

6.**会议名称：**ACM MULTIMEDIA CONFERENCE 2020

会议时间：12-16 October 2020

会议地点：Seattle, United States

会议简介：2020-4-21

With numerous requests from the multimedia community, we decide to further extend the deadline for regular papers to 5/24 with the following timeline thereafter. We hope this will give those authors from the areas heavily impacted by the COVID-19 outbreak more time to prepare for their submissions.

5/17 submission deadline for abstracts

5/24 submission deadline for regular papers

7/1-7/5 rebuttal period

7/25 notification

8/10 camera-ready for regular papers

All other tracks (workshops, challenges, tutorials, demo & video, brave new topics, etc.) may adjust the timeline accodingly based on the preparation schedule by ACM publisher at http://www.scomminc.com/pp/schedules/MM20-ACM-DL-only-schedule.htm.

链接：https://2020.acmmm.org/

7.**会议名称：**CIPAE 2020

会议时间：October 16-18, 2020

会议地点：Ottawa, Canada

会议简介：2020 International Conference on Computers, Information Processing and Advanced Education (CIPAE 2020) will take place in Ottawa, Canada, on October 16-18, 2020. CIPAE 2020 seeks to provide a high-level forum for experts, researchers, professionals, innovators and

practitioners in the field of computers, information processing and advanced education. It will attract industry and academia to present and discuss the wide spectrum of original and novel researches and contributions together.

computers, information processing and advanced education are hotspot topics in modern academic and scientific field. They represent especially new research direction, so novel and state-of-the-art researches and inventions related to computers, information processing and advanced education emerge continuously. Besides, computers, information processing and advanced educationcan be widely applied in many fields, such as computer networks, computer security, approximate computing, computer performance, computer applications, computer architecture, computer interfaces, computer peripherals, data systems, digital systems, distributed computing, image processing, parallel processing, software engineering, adaptive learning, educational technology, engineering education, training and so on. Therefore, CIPAE 2020 will serve as a catalyst for explorations and discussion on new concepts and novel achievements of computers, information processing and advanced education, with applications from theoretical research and practical applications at the same time.

All papers related to vomputers, information processing and advanced education and their applications are solicited and welcomed for oral presentation or poster presentation or virtual presentation at the conference. Accepted papers will be published in International Conference Proceedings, which will be submitted for index by Ei Compendex, Scopus, WoS, etc. CIPAE 2020 is sponsored by Institute of Electronics and Computer (IEC) and technically assisted by many universities and institutes. On behalf of the organizing committee, we cordially express our appreciation to the international organization committee, technical committee and attendees of the international event. It is hoped that this international conference will be a precious opportunity for you to exchange scientific ideas, inspire new research and new contacts for closer cooperation, so we can envisage the future of a promising development of computers, information processing and advanced education.

链接：http://cipae.net/index.html

8.**会议名称：**SPLASH 2020

会议时间：Sun 15 - Fri 20 November 2020

会议地点：Chicago, USA

会议简介：SPLASH is the ACM SIGPLAN conference on Systems, Programming, Languages, and Applications: Software for Humanity. SPLASH embraces all aspects of software construction and delivery, to make it the premier conference on the applications of programming languages—at the intersection of programming languages and software engineering. SPLASH 2020 will take place in Chicago from Sunday 15th to Friday 20th of November 2020. Early registration deadline for the conference will be Thursday 15th October AOE.

SPLASH includes the following co-located conferences: OOPSLA, Onward!, GPCE, SLE, DLS, and SAS; as well as a large array of workshops and events.

The SPLASH-I will feature a number of speakers of interest to software practitioners and researchers alike.

链接：https://conf.researchr.org/home/splash-2020

9.会议名称：BuildSys 2020
会议时间：November 16-19, 2020
会议地点：Yokohama, Japan
会议简介：The 7th ACM International Conference on Systems for Energy-Efficient Built Environments (BuildSys 2020) will host a highly selective, single-track forum for research on systems issues covering all aspects of the built environment, broadly defined.
Advances in the effective integration of networked sensors, building controls, and physical infrastructure are transforming our society, allowing the formation of unprecedented built environments and interlocking physical, social, cyber challenges. Moreover, built environments, including buildings and critical urban infrastructure, account for over half of societys energy consumption and are the mainstay of our nation’s economy, security and health. As a result, there is a broad recognition that systems optimizing explicitly for the built environment are particularly important in improving our society, and represent the foundation for emerging "smart cities".
BuildSys is an ideal venue for researchers and practitioners working to develop and optimize such smart infrastructure systems that are driven by networked sensing, computing, and control functions.
链接：http://buildsys.acm.org/2020/

10.会议名称：SCAI 2020
会议时间：19-20 December, 2020
会议地点：Sydney, Australia
会议简介：9th International Conference on Soft Computing, Artificial Intelligence and Applications (SCAI 2020) will provide an excellent international forum for sharing knowledge and results in theory, methodology and applications of artificial intelligence, soft computing. The conference looks for significant contributions to all major fields of the artificial intelligence, soft computing in theoretical and practical aspects. The aim of the conference is to provide a platform to the researchers and practitioners from both academia as well as industry to meet and share cutting-edge development in the field.
Authors are solicited to contribute to the conference by submitting articles that illustrate research results, projects, surveying works and industrial experiences that describe significant advances in the following areas, but are not limited to.
链接：https://iccsea2020.org/scai/index.html

IQPC 最新国防会议(Defence)

IQPC 来源：http://www.iqpc.com/

1. **会议名称：**Future Artillery
会议时间：27 - 29 October, 2020
会议地点：Twickenham Stadium, London, United Kingdom
会议简介：It is no coincidence that the fielding of a long-range precision fires capability tops the US Army's list of modernisation priorities. The importance of artillery as a joint enabler has been consistently underlined by concepts of operation that describe a contested future battlespace – where the predominance of A2/AD technologies deny the air superiority on which NATO has come to rely.
The Future Artillery conference remains the premier platform for discussing those next-generation systems that will provide a decisive long-range fires capability for future multi-domain operations. New in 2020, the conference will look not just at the systems themselves, but at the network and ISTAR enterprise that will be integral to applying fires in the future land and joint environment. It provides an opportunity for 200 defence and industry leaders from more than 20 countries to gather and overcome shared challenges relating to future force design, training, capability and – perhaps most importantly – interoperability.
链接：https://www.defenceiq.com/events-futureartillery/?utm_medium=portal&mac=IQPCCORP

2.**会议名称：**Land Forces Training
会议时间：28 - 29 October, 2020
会议地点：London, UK
会议简介：As land power doctrine re-orientates towards multi-domain operations there is a need to invest in new training capabilities that will develop adaptive and innovative soldiers, capable of fighting against skilled enemies and winning in complex, changing battlespaces.
This change is part of a broader strategic modernisation initiative reshaping army thinking today, driven largely by two key factors: technology and a vision of the future operating environment.
The inaugural Land Forces Training conference will fuse the best of industry with eclectic sources of military expertise to build meaningful consensus across coalitions and industry partnerships on the training needs of the future warfighter - providing a forum for discussion on what skills will be required to fight and win in 2050.
链接：
https://www.defenceiq.com/events-landforcestraining/?utm_medium=portal&mac=IQPCCORP

3.**会议名称：**CABSEC/SAMSEC
会议时间：03 - 05 November, 2020
会议地点：Club Naval, Cartagena, Colombia
会议简介：Defence IQ's 8th annual CABSEC and SAMSEC, hosted by the Colombia Navy in Cartagena de Indias, has been postponed until 3 - 5 November 2020.
This established forum meets annually and brings together the region's defence and security

leadership to discuss strategy, cooperation, requirements and challenges and has helped advance the security dialogue in the region through the forum's objectives to;

Promote regional and hemispheric security cooperation through expanding networks

Help to build enduring partnerships in order to enhance regional security capacity in Central and South America and the Caribbean

The theme for 2020 is Increasing the Impact of International Cooperation on Transnational Crime. The Colombian Navy will host our international delegations to take part in discussions, debates and networking including bi-lateral meetings in order to enhance cooperation and establish meaningful consensus on shared challenges. We will also give attendees the unique opportunity to to experience the rich Naval tradition of Cartagena and visit some of the facilities around the bay area. Participants will visit the International Centre Against Drug Trafficking (CIMCON) and the International Coast Guard School within the Naval School (ENAP), COTECMAR and the Colombian Naval Base in Cartagena.

Industry is welcome to join the forum and raise awareness of the technical solutions available to the many challenges across the region.

链接：https://www.defenceiq.com/events-cabsec/?utm_medium=portal&mac=IQPCCORP

4.**会议名称：**Warships & OPV Latin America

会议时间：10 - 12 November, 2020

会议地点：Lima Peru

会议简介：The Warships & OPV Latin America Conference is a forum for discussion on ship design priorities and emerging requirements to strengthen fleet versatility and retain high readiness for the full spectrum of maritime operations. Given the commonality of maritime hemispheric challenges, the conference examines cost-effective ways to manage the renewal and acquisition of naval platforms with updated technologies, advance multi-mission modularity, and enhance indigenous shipbuilding capability. As an international strategic platform, it offers a comprehensive account of geostrategic issues shaping doctrine and requirements for the future fleet and facilitates dialogue between navies, coast guards, national shipyards, and industry.

Over the course of 3 days, the event will address operational requirements for current operations, anticipated platform modernisation and ongoing procurement plans, as well as emerging requirements for specialist vessels.

Since its inception in 2012, the Warships & OPV Latin America conference has grown to become the premier meeting ground for the Higher Naval Commands of the region, attracting over 150 senior officials including Navy Commanders, Directors of Materiel, Heads of Strategic Programs, capability planners, shipyard Directors, as well as leading solution providers. Previous meetings were hosted by Brazil (2018) Chile (2017), Peru (2016), Ecuador (2015), Colombia (2014) and Brazil (2012 and 2013).

链接：https://www.defenceiq.com/events-opvlatam/?utm_medium=portal&mac=IQPCCORP

5.**会议名称：**International Fighter

会议时间：18 - 20 November, 2020

会议地点：Hilton Berlin, Germany

会议简介：The International Fighter Conference 2019 returns to Berlin to discuss the future of

Combat Air Power across the spectrum of operations. The utility of Combat Air, air-integration into multi-domain operations, and continuing interest in both next generation and light attack platforms calls for a broad range of discussion suited to the 250 attendees that gather each year from both large and small air forces alike. The Conference, now in its 19th year, has built a reputation as the world's premier event for all elements of the fighter aircraft community, with attendance spanning from the Americas, Europe, the Middle East and parts of Asia.

Investment in expensive high-end platforms needs to be balanced with a requirement for platforms adept and efficient in low-intensity conflict. What is consistent is that information and connectivity is at the heart of operations. This year's wide-ranging programme uniquely covers the key and emerging issues related to airpower delivery for military leaders and industry. Over the few conference days, we will exchange perspectives and gain insights towards meeting the challenges of operations now and in the future, addressing integration of next generation assets with existing platforms, light attack aircraft, electro-magnetic spectrum dominance, cyber integration, advanced training, LVC, cost-effective capability development, disruptive technologies and mission planning. The next generation programmes, including FCAS, Tempest, and F-X will be discussed and will provide an incredible opportunity to revolutionise airpower delivery and open the door for international opportunities.

The conference format runs 12-14 November with the 14 November comprising a day of focus sessions: a dedicated morning for smaller air forces to examine the Ford vs. Ferrari debate and a focus afternoon, evaluating the role of disruptive technologies in future airpower delivery.

链接：

https://www.defenceiq.com/events-internationalfighter/?utm_medium=portal&mac=IQPCCORP

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