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

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

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

如果您对我们的栏目设置、内容编排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

2021 年 3 月

目 录

Nature Latest Research (Chemistry)

来源：https://www.nature.com/nphys/research

1. **标题：**Mechanism of mediated alkali peroxide oxidation and triplet versus singlet oxygen formation

作者：Yann K. Petit, Eléonore Mourad, Christian Prehal, Christian Leypold, Andreas Windischbacher, Daniel Mijailovic, Christian Slugovc, Sergey M. Borisov, Egbert Zojer, Sergio Brutti, Olivier Fontaine & Stefan A. Freunberger

摘要：Aprotic alkali metal–O2 batteries face two major obstacles to their chemistry occurring efficiently, the insulating nature of the formed alkali superoxides/peroxides and parasitic reactions that are caused by the highly reactive singlet oxygen (1O2). Redox mediators are recognized to be key for improving rechargeability. However, it is unclear how they affect 1O2 formation, which hinders strategies for their improvement. Here we clarify the mechanism of mediated peroxide and superoxide oxidation and thus explain how redox mediators either enhance or suppress 1O2 formation. We show that charging commences with peroxide oxidation to a superoxide intermediate and that redox potentials above ~3.5 V versus Li/Li+ drive 1O2 evolution from superoxide oxidation, while disproportionation always generates some 1O2. We find that 1O2 suppression requires oxidation to be faster than the generation of 1O2 from disproportionation. Oxidation rates decrease with growing driving force following Marcus inverted-region behaviour, establishing a region of maximum rate.

链接：https://www.nature.com/articles/s41557-021-00643-z

2. **标题：**O-GlcNAc modification of small heat shock proteins enhances their anti-amyloid chaperone activity

作者：Aaron T. Balana, Paul M. Levine, Timothy W. Craven, Somnath Mukherjee, Nichole J. Pedowitz, Stuart P. Moon, Terry T. Takahashi, Christian F. W. Becker, David Baker & Matthew R. Pratt

摘要：A major role for the intracellular post-translational modification O-GlcNAc appears to be the inhibition of protein aggregation. Most of the previous studies in this area focused on O-GlcNAc modification of the amyloid-forming proteins themselves. Here we used synthetic protein chemistry to discover that O-GlcNAc also activates the anti-amyloid activity of certain small heat shock proteins (sHSPs), a potentially more important modification event that can act broadly and substoichiometrically. More specifically, we found that O-GlcNAc increases the ability of sHSPs to block the amyloid formation of both α-synuclein and Aβ(1–42). Mechanistically, we show that O-GlcNAc near the sHSP IXI-domain prevents its ability to intramolecularly compete with substrate binding. Finally, we found that, although O-GlcNAc levels are globally reduced in Alzheimer’s disease brains, the modification of relevant sHSPs is either maintained or increased, which suggests a mechanism to maintain these potentially protective O-GlcNAc modifications. Our results have important implications for

neurodegenerative diseases associated with amyloid formation and potentially other areas of sHSP biology.

链接：https://www.nature.com/articles/s41557-021-00648-8

3. **标题：**Stereoelectronic effects in stabilizing protein–N-glycan interactions revealed by experiment and machine learning

作者：Maziar S. Ardejani, Louis Noodleman, Evan T. Powers & Jeffery W. Kelly

摘要：The energetics of protein–carbohydrate interactions, central to many life processes, cannot yet be manipulated predictably. This is mostly due to an incomplete quantitative understanding of the enthalpic and entropic basis of these interactions in aqueous solution. Here, we show that stereoelectronic effects contribute to stabilizing protein–N-glycan interactions in the context of a cooperatively folding protein. Double-mutant cycle analyses of the folding data from 52 electronically varied N-glycoproteins demonstrate an enthalpy–entropy compensation depending on the electronics of the interacting side chains. Linear and nonlinear models obtained using quantum mechanical calculations and machine learning explain up to 79% and 97% of the experimental interaction energy variability, as inferred from the R2 value of the respective models. Notably, the protein–carbohydrate interaction energies strongly correlate with the molecular orbital energy gaps of the interacting substructures. This suggests that stereoelectronic effects must be given a greater weight than previously thought for accurately modelling the short-range dispersive van der Waals interactions between the N-glycan and the protein.

链接：https://www.nature.com/articles/s41557-021-00646-w

4. **标题：**Reagentless biomolecular analysis using a molecular pendulum

作者：Jagotamoy Das, Surath Gomis, Jenise B. Chen, Hanie Yousefi, Sharif Ahmed, Alam Mahmud, Wendi Zhou, Edward H. Sargent & Shana O. Kelley

摘要：The development of reagentless sensors that can detect molecular analytes in biological fluids could enable a broad range of applications in personalized health monitoring. However, only a limited set of molecular inputs can currently be detected using reagentless sensors. Here, we report a sensing mechanism that is compatible with the analysis of proteins that are important physiological markers of stress, allergy, cardiovascular health, inflammation and cancer. The sensing method is based on the motion of an inverted molecular pendulum that exhibits field-induced transport modulated by the presence of a bound analyte. We measure the sensor's electric field-mediated transport using the electron-transfer kinetics of an attached reporter molecule. Using time-resolved electrochemical measurements that enable unidirectional motion of our sensor, the presence of an analyte bound to our sensor complex can be tracked continuously in real time. We show that this sensing approach is compatible with making measurements in blood, saliva, urine, tears and sweat and that the sensors can collect data in situ in living animals.

链接：https://www.nature.com/articles/s41557-021-00644-y

5. **标题：**Metathesis of Ge=Ge double bonds

作者：Lukas Klemmer, Anna-Lena Thömmes, Michael Zimmer, Volker Huch, Bernd Morgenstern & David Scheschkewitz

摘要：The metathesis of carbon–carbon double bonds—the 'reshuffling' of their constituting

carbene fragments—is a tremendously important preparative tool in industry and academia. Metathesis of heavier alkene homologues is restricted to occasional unproductive examples in phosphorus chemistry and cross-metathesis to mixed heavier alkynes. We now report the thermally induced, transition-metal-free metathesis of purpose-built unsymmetrically substituted digermenes. The A2Ge=GeAB starting materials are thus converted to symmetrically substituted derivatives of the A2Ge=GeA2 and ABGe=GeAB types. The use of tethered auxiliary donors (dimethylaniline groups) in substituents B ensures intramolecular donor–acceptor stabilization of the transient germylene fragments, the intermediacy of which is proven by trapping experiments. Density functional theory calculations shed light on the thermodynamic driving force of the metathesis and validate the crucial role of the tethered donor. With an analogously equipped bridged tetragermadiene precursor (A2Ge=GeB-X-BGe=GeA2), heavier acyclic diene metathesis polymerization occurs, in analogy to the widespread acyclic diene metathesis (ADMET) polymerization in the carbon case, yielding a polydigermene.

链接：https://www.nature.com/articles/s41557-021-00639-9

6. **标题：**Abiotic reduction of ketones with silanes catalysed by carbonic anhydrase through an enzymatic zinc hydride

作者：Pengfei Ji, Jeeyoung Park, Yang Gu, Douglas S. Clark & John F. Hartwig

摘要：Enzymatic reactions through mononuclear metal hydrides are unknown in nature, despite the prevalence of such intermediates in the reactions of synthetic transition-metal catalysts. If metalloenzymes could react through abiotic intermediates like these, then the scope of enzyme-catalysed reactions would expand. Here we show that zinc-containing carbonic anhydrase enzymes catalyse hydride transfers from silanes to ketones with high enantioselectivity. We report mechanistic data providing strong evidence that the process involves a mononuclear zinc hydride. This work shows that abiotic silanes can act as reducing equivalents in an enzyme-catalysed process and that monomeric hydrides of electropositive metals, which are typically unstable in protic environments, can be catalytic intermediates in enzymatic processes. Overall, this work bridges a gap between the types of transformation in molecular catalysis and biocatalysis.

链接：https://www.nature.com/articles/s41557-020-00633-7

7. **标题：**Co-precipitation behaviour of single atoms of rutherfordium in basic solutions

作者：Yoshitaka Kasamatsu, Keigo Toyomura, Hiromitsu Haba, Takuya Yokokita, Yudai Shigekawa, Aiko Kino, Yuki Yasuda, Yukiko Komori, Jumpei Kanaya, Minghui Huang, Masashi Murakami, Hidetoshi Kikunaga, Eisuke Watanabe, Takashi Yoshimura, Kosuke Morita, Toshiaki Mitsugashira, Koichi Takamiya, Tsutomu Ohtsuki & Atsushi Shinohara

摘要：All superheavy elements (SHEs), with atomic numbers (Z) ≥104, have been artificially synthesized one atom at a time and their chemical properties are largely unknown. Because these heavy nuclei have short lifetimes as well as extremely low production rates, chemical experiments need to be carried out on single atoms and have mostly been limited to adsorption and extraction. We have now investigated the precipitation properties of the SHE Rf (Z = 104). A co-precipitation method with samarium hydroxide had previously established that the co-precipitation behaviour of a range of elements reflected these elements' tendency to form hydroxide precipitates and/or ammine complex ions. Here we investigated co-precipitation of Rf in basic solutions containing

NH3 or NaOH. Comparisons between the behaviour of Rf with that of Zr and Hf (lighter homologues of Rf) and actinide Th (a pseudo-homologue of Rf) showed that Rf does not coordinate strongly with NH3, but forms a hydroxide (co)precipitate that is expected to be Rf(OH)4.

链接：https://www.nature.com/articles/s41557-020-00634-6

8. **标题：**Dipolar order in an amphidynamic crystalline metal–organic framework through reorienting linkers

作者：Y.-S. Su, E. S. Lamb, I. Liepuoniute, A. Chronister, A. L. Stanton, P. Guzman, S. Pérez-Estrada, T. Y. Chang, K. N. Houk, M. A. Garcia-Garibay & S. E. Brown

摘要：Amphidynamic crystals, which possess crystallinity and support dynamic behaviours, are very well suited to the exploration of emergent phenomena that result from the coupling on the dynamic moieties. Here, dipolar rotors have been embedded in a crystalline metal–organic framework. The material consists of Zn(II) nodes and two types of ditopic bicyclo[2.2.2]octane-based linkers—one that coordinates to the Zn clusters through two 1,4-aza moieties, and a difluoro-functionalized derivative (the dipolar rotor) that coordinates through linked 1,4-dicarboxylate groups instead. Upon cooling, these linkers collectively order as a result of correlated dipole–dipole interactions. Variable-temperature, frequency-dependent dielectric measurements revealed a transition temperature Tc = 100 K, when a rapidly rotating, dipole-disordered, paraelectric phase transformed into an ordered, antiferroelectric one in which the dipole moments of the rotating linkers largely cancelled each other. Monte Carlo simulations on a two-dimensional rotary lattice showed a ground state with an Ising symmetry and the effects of dipole–lattice and dipole–dipole interactions.

链接：https://www.nature.com/articles/s41557-020-00618-6

9. **标题：**Illuminating the dark conformational space of macrocycles using dominant rotors

作者：Diego B. Diaz, Solomon D. Appavoo, Anastasia F. Bogdanchikova, Yury Lebedev, Timothy J. McTiernan, Gabriel dos Passos Gomes & Andrei K. Yudin

摘要：Three-dimensional conformation is the primary determinant of molecular properties. The thermal energy available at room temperature typically equilibrates the accessible conformational states. Here, we introduce a method for isolating unique and previously understudied conformations of macrocycles. The observation of unusual conformations of 16- to 22-membered rings has been made possible by controlling their interconversion using dominant rotors, which represent tunable atropisomeric constituents with relatively high rotational barriers. Density functional theory and in situ NMR measurements suggest that dominant rotor candidates for the amino-acid-based structures considered here should possess a rotational energy barrier of at least 25 kcal mol−1. Notable differences in the geometries of the macrocycle conformations were identified by NMR spectroscopy and X-ray crystallography. There is evidence that amino acid residues can be forced into rare turn motifs not observed in the corresponding linear counterparts and homodetic rings. These findings should unlock new avenues for studying the conformation–activity relationships of bioactive molecules.

链接：https://www.nature.com/articles/s41557-020-00620-y

10. **标题：**Metal–organic frameworks embedded in a liposome facilitate overall photocatalytic water splitting

作者：Huihui Hu, Zhiye Wang, Lingyun Cao, Lingzhen Zeng, Cankun Zhang, Wenbin Lin & Cheng Wang

摘要：Metal–organic frameworks (MOFs) have been studied extensively in the hydrogen evolution reaction (HER) and the water oxidation reaction (WOR) with sacrificial reagents, but overall photocatalytic water splitting using MOFs has remained challenging, principally because of the fast recombination of photo-generated electrons and holes. Here we have integrated HER- and WOR-MOF nanosheets into liposomal structures for separation of the generated charges. The HER-MOF nanosheets comprise light-harvesting Zn–porphyrin and catalytic Pt–porphyrin moieties, and are functionalized with hydrophobic groups to facilitate their incorporation into the hydrophobic lipid bilayer of the liposome. The WOR-MOF flakes consist of [Ru(2,2′-bipyridine)3]2+-based photosensitizers and Ir–bipyridine catalytic centres, and are localized in the hydrophilic interior of the liposome. This liposome–MOF assembly achieves overall photocatalytic water splitting with an apparent quantum yield of (1.5 ± 1)% as a result of ultrafast electron transport from the antennae (Zn–porphyrin and [Ru(2,2′-bipyridine)3]2+) to the reaction centres (Pt–porphyrin and Ir–bipyridine) in the MOFs and efficient charge separation in the lipid bilayers.

链接：https://www.nature.com/articles/s41557-020-00635-5

11. **标题：**Predicting the stability of homotrimeric and heterotrimeric collagen helices

作者：Douglas R. Walker, Sarah A. H. Hulgan, Caroline M. Peterson, I-Che Li, Kevin J. Gonzalez & Jeffrey D. Hartgerink

摘要：Robust methods for predicting thermal stabilities of collagen triple helices are critical for understanding natural structure and stability in the collagen family of proteins and also for designing synthetic peptides mimicking these essential proteins. In this work, we determine the relative stability imparted on the collagen triple helix by single amino acids and interactions between amino acid pairs. Using this analysis, we create a comprehensive algorithm, SCEPTTr, for predicting melting temperatures of synthetic triple helices. Critically, our algorithm is compatible with every natural amino acid, can evaluate both homotrimers and heterotrimers, and accounts for all possible helix compositions and registers, including non-canonically staggered helices. We test and optimize our algorithm against 431 published collagen triple helices to demonstrate the quality of our predictive system. Finally, we use this algorithm to successfully guide the design of an ABC heterotrimer possessing high assembly specificity.

链接：https://www.nature.com/articles/s41557-020-00626-6

12. **标题：**Direct observation of coherent femtosecond solvent reorganization coupled to intramolecular electron transfer

作者：Elisa Biasin, Zachary W. Fox, Amity Andersen, Kathryn Ledbetter, Kasper S. Kjær, Roberto Alonso-Mori, Julia M. Carlstad, Matthieu Chollet, James D. Gaynor, James M. Glownia, Kiryong Hong, Thomas Kroll, Jae Hyuk Lee, Chelsea Liekhus-Schmaltz, Marco Reinhard, Dimosthenis Sokaras, Yu Zhang, Gilles Doumy, Anne Marie March, Stephen H. Southworth, Shaul Mukamel, Kelly J. Gaffney, Robert W. Schoenlein, Niranjan Govind, Amy A. Cordones & Munira Khalil

摘要：It is well known that the solvent plays a critical role in ultrafast electron-transfer reactions. However, solvent reorganization occurs on multiple length scales, and selectively measuring short-range solute–solvent interactions at the atomic level with femtosecond time resolution remains a challenge. Here we report femtosecond X-ray scattering and emission measurements following photoinduced charge-transfer excitation in a mixed-valence bimetallic (FeIIRuIII) complex in water, and their interpretation using non-equilibrium molecular dynamics simulations. Combined experimental and computational analysis reveals that the charge-transfer excited state has a lifetime of 62 fs and that coherent translational motions of the first solvation shell are coupled to the back electron transfer. Our molecular dynamics simulations identify that the observed coherent translational motions arise from hydrogen bonding changes between the solute and nearby water molecules upon photoexcitation, and have an amplitude of tenths of ångströms, 120–200 cm−1 frequency and ~100 fs relaxation time. This study provides an atomistic view of coherent solvent reorganization mediating ultrafast intramolecular electron transfer.
链接：https://www.nature.com/articles/s41557-020-00629-3

13. **标题：**The photochemical reaction of phenol becomes ultrafast at the air–water interface
作者：Ryoji Kusaka, Satoshi Nihonyanagi & Tahei Tahara
摘要：Reactions at the interface between water and other phases play important roles in nature and in various chemical systems. Although some experimental and theoretical studies suggest that chemical reactions at water interfaces can be different from those in bulk water—for example, 'on-water catalysis' and the activation of photochemically inert fatty acids at the air–water interface upon photoexcitation—directly investigating these differences and generating molecular-level understanding has proved difficult. Here, we report on the direct probing of a photochemical reaction occurring at the air–water interface, using ultrafast phase-sensitive interface-selective nonlinear vibrational spectroscopy. The femtosecond time-resolved data obtained clearly show that the photoionization reaction of phenol proceeds 104 times faster at the water surface than in the bulk aqueous phase (upon irradiation with photons with the same energy). This finding demonstrates that photochemical reactions at water interfaces are very different from those in bulk water, reflecting distinct reaction environments at the interface.
链接：https://www.nature.com/articles/s41557-020-00619-5

14. **标题：**Efficient Lewis acid catalysis of an abiological reaction in a de novo protein scaffold
作者：Sophie Basler, Sabine Studer, Yike Zou, Takahiro Mori, Yusuke Ota, Anna Camus, H. Adrian Bunzel, Roger C. Helgeson, K. N. Houk, Gonzalo Jiménez-Osés & Donald Hilvert
摘要：New enzyme catalysts are usually engineered by repurposing the active sites of natural proteins. Here we show that design and directed evolution can be used to transform a non-natural, functionally naive zinc-binding protein into a highly active catalyst for an abiological hetero-Diels–Alder reaction. The artificial metalloenzyme achieves >104 turnovers per active site, exerts absolute control over reaction pathway and product stereochemistry, and displays a catalytic proficiency ($1/K_{TS} = 2.9 \times 10^{10}$ M−1) that exceeds all previously characterized Diels–Alderases. These properties capitalize on effective Lewis acid catalysis, a chemical strategy for accelerating Diels–Alder reactions common in the laboratory but so far unknown in nature. Extension of this approach to other metal ions and other de novo scaffolds may propel the design field in exciting

new directions.

链接：https://www.nature.com/articles/s41557-020-00628-4

15. **标题：**Palladium-catalysed carboformylation of alkynes using acid chlorides as a dual carbon monoxide and carbon source

作者：Yong Ho Lee, Elliott H. Denton & Bill Morandi

摘要：Hydroformylation, a reaction that installs both a C–H bond and an aldehyde group across an unsaturated substrate, is one of the most important catalytic reactions in both industry and academia. Given the synthetic importance of creating new C–C bonds, the development of carboformylation reactions, wherein a new C–C bond is formed instead of a C–H bond, would bear enormous synthetic potential to rapidly increase molecular complexity in the synthesis of valuable aldehydes. However, the demanding complexity inherent in a four-component reaction, utilizing an exogenous CO source, has made the development of a direct carboformylation reaction a formidable challenge. Here, we describe a palladium-catalysed strategy that uses readily available aroyl chlorides as a carbon electrophile and CO source, in tandem with a sterically congested hydrosilane, to perform a stereoselective carboformylation of alkynes. An extension of this protocol to four chemodivergent carbonylations further highlights the creative opportunity offered by this strategy in carbonylation chemistry.

链接：https://www.nature.com/articles/s41557-020-00621-x

16. **标题：**Mechanochemical bond scission for the activation of drugs

作者：Shuaidong Huo, Pengkun Zhao, Zhiyuan Shi, Miancheng Zou, Xintong Yang, Eliza Warszawik, Mark Loznik, Robert Göstl & Andreas Herrmann

摘要：Pharmaceutical drug therapy is often hindered by issues caused by poor drug selectivity, including unwanted side effects and drug resistance. Spatial and temporal control over drug activation in response to stimuli is a promising strategy to attenuate and circumvent these problems. Here we use ultrasound to activate drugs from inactive macromolecules or nano-assemblies through the controlled scission of mechanochemically labile covalent bonds and weak non-covalent bonds. We show that a polymer with a disulfide motif at the centre of the main chain releases an alkaloid-based anticancer drug from its β-carbonate linker by a force-induced intramolecular 5-exo-trig cyclization. Second, aminoglycoside antibiotics complexed by a multi-aptamer RNA structure are activated by the mechanochemical opening and scission of the nucleic acid backbone. Lastly, nanoparticle–polymer and nanoparticle–nanoparticle assemblies held together by hydrogen bonds between the peptide antibiotic vancomycin and its complementary peptide target are activated by force-induced scission of hydrogen bonds. This work demonstrates the potential of ultrasound to activate mechanoresponsive prodrug systems.

链接：https://www.nature.com/articles/s41557-020-00624-8

17. **标题：**Synthesis of a zigzag carbon nanobelt

作者：Kwan Yin Cheung, Kosuke Watanabe, Yasutomo Segawa & Kenichiro Itami

摘要：The structure-selective precise synthesis of carbon nanotubes (CNTs) has been long sought in materials science. The aromatic molecules corresponding to segment structures of CNTs, that is, carbon nanobelts (CNBs), are of interest as templates for CNT growth. Among the three types of

CNB (armchair, chiral and zigzag CNBs), zigzag CNBs have been considered the most difficult type to synthesize. Here we report the synthesis, isolation and structural characterization of a zigzag CNB. The synthesis involves an iterative Diels–Alder reaction sequence followed by reductive aromatization of oxygen-bridged moieties. As predicted by theoretical calculations, this CNB was isolated as a stable compound. The structure of the zigzag CNB was fully characterized by X-ray crystallography and its wide energy gap with blue fluorescence properties was revealed by photophysical measurements. With synthetic strategies towards all three types of CNB in hand, the road to the precise synthesis of CNTs can now proceed to the next stage.

链接：https://www.nature.com/articles/s41557-020-00627-5

18. **标 题 ：** Iron-catalysed synthesis and chemical recycling of telechelic 1,3-enchained oligocyclobutanes

作者：Megan Mohadjer Beromi, C. Rose Kennedy, Jarod M. Younker, Alex E. Carpenter, Sarah J. Mattler, Joseph A. Throckmorton & Paul J. Chirik

摘要：Closed-loop recycling offers the opportunity to mitigate plastic waste through reversible polymer construction and deconstruction. Although examples of chemical recycling of polymers are known, few have been applied to materials derived from abundant commodity olefinic monomers, which are the building blocks of ubiquitous plastic resins. Here we describe a [2+2] cycloaddition/oligomerization of 1,3-butadiene to yield a previously unrealized telechelic microstructure of (1,n′-divinyl)oligocyclobutane. This material is thermally stable, has stereoregular segments arising from chain-end control, and exhibits high crystallinity even at low molecular weight. Exposure of the oligocyclobutane to vacuum in the presence of the pyridine(diimine) iron precatalyst used to synthesize it resulted in deoligomerization to generate pristine butadiene, demonstrating a rare example of closed-loop chemical recycling of an oligomeric material derived from a commodity hydrocarbon feedstock.

链接：https://www.nature.com/articles/s41557-020-00614-w

19. **标题：**Quasiclassical simulations based on cluster models reveal vibration-facilitated roaming in the isomerization of CO adsorbed on NaCl

作者：Apurba Nandi, Peng Zhang, Jun Chen, Hua Guo & Joel M. Bowman

摘要：The desire to better understand the quantum nature of isomerization led to recent experimental observations of the vibrationally induced isomerization of OC–NaCl(100) to CO–NaCl(100). To investigate the mechanism of this isomerization, we performed dynamics calculations using finite (CO–NaCl)n cluster models. We constructed new potential energy surfaces for CO–NaCl and CO–CO interactions using high-level ab initio data and report key properties of the bare CO–NaCl potential energy surface, which show much in common with the experiment. We investigated the isomerization dynamics using several cluster models and, in all cases, isomerization was seen for highly excited CO vibrational states, in agreement with experiments. A detailed examination of the reaction trajectories indicates that isomerization occurs when the distance between CO and NaCl is larger than the distance at the conventional isomerization saddle point, which is a strong indicator of ‘roaming’.

链接：https://www.nature.com/articles/s41557-020-00612-y

20. **标题：**Quaternary stereocentres via catalytic enantioconvergent nucleophilic substitution reactions of tertiary alkyl halides

作者：Zhaobin Wang, Ze-Peng Yang & Gregory C. Fu

摘要：The development of efficient methods, particularly catalytic and enantioselective processes, for the construction of all-carbon quaternary stereocentres is an important (and difficult) challenge in organic synthesis due to the occurrence of this motif in a range of bioactive molecules. One conceptually straightforward and potentially versatile approach is the catalytic enantioconvergent substitution reaction of a readily available racemic tertiary alkyl electrophile by an organometallic nucleophile; however, examples of such processes are rare. Here we demonstrate that a nickel-based chiral catalyst achieves enantioconvergent couplings of a variety of tertiary electrophiles (cyclic and acyclic α-halocarbonyl compounds) with alkenylmetal nucleophiles to form quaternary stereocentres with good yield and enantioselectivity under mild conditions in the presence of a range of functional groups. These couplings, which probably proceed via a radical pathway, provide access to an array of useful families of organic compounds, including intermediates in the total synthesis of two natural products, (−)-eburnamonine and madindoline A.

链接：https://www.nature.com/articles/s41557-020-00609-7

IEL Top25

（来源：http://ieeexplore.ieee.org/）

1.标题：Phantom Malware: Conceal Malicious Actions From Malware Detection Techniques by Imitating User Activity
出处： IEEE Access
作者：Tim Niklas Witte
摘要：State of the art malware detection techniques only consider the interaction of programs with the operating system's API (system calls) for malware classification. This paper demonstrates that techniques like these are insufficient. A point that is overlooked by the currently existing techniques is presented in this paper: Malware is able to interact with windows providing the corresponding functionality in order to execute the desired action by mimicking user activity. In other words, harmful actions will be masked as simulated user actions. To start with, the article introduces User Imitating techniques for concealing malicious commands of the malware as impersonated user activity. Thereafter, the concept of Phantom Malware will be presented: This malware is constantly applying User Imitating to execute each of its malicious actions. A Phantom Ransomware (ransomware employs the User Imitating for every of its malicious actions) is implemented in C++ for testing anti-virus programs in Windows 10. Software of various manufacturers are applied for testing purposes. All of them failed without exception. This paper analyzes the reasons why these products failed and further, presents measures that have been developed against Phantom Malware based on the test results.
链接：https://ieeexplore.ieee.org/document/9186656

2.标题：Artificial Intelligence and COVID-19: Deep Learning Approaches for Diagnosis and Treatment
出处： IEEE Access
作者：Mohammad Jamshidi;Ali Lalbakhsh;Jakub Talla;Zdeněk Peroutka;Farimah Hadjilooei;Pedram Lalbakhsh;Morteza Jamshidi;Luigi La Spada;Mirhamed Mirmozafari;Mojgan Dehghani;Asal Sabet;Saeed Roshani;Sobhan Roshani;Nima Bayat-Makou;Bahare Mohamadzade;Zahra Malek;Alireza Jamshidi;Sarah Kiani;Hamed Hashemi-Dezaki;Wahab Mohyuddin
摘要：COVID-19 outbreak has put the whole world in an unprecedented difficult situation bringing life around the world to a frightening halt and claiming thousands of lives. Due to COVID-19's spread in 212 countries and territories and increasing numbers of infected cases and death tolls mounting to 5,212,172 and 334,915 (as of May 22 2020), it remains a real threat to the public health system. This paper renders a response to combat the virus through Artificial Intelligence (AI). Some Deep Learning (DL) methods have been illustrated to reach this goal, including Generative Adversarial Networks (GANs), Extreme Learning Machine (ELM), and

Long/Short Term Memory (LSTM). It delineates an integrated bioinformatics approach in which different aspects of information from a continuum of structured and unstructured data sources are put together to form the user-friendly platforms for physicians and researchers. The main advantage of these AI-based platforms is to accelerate the process of diagnosis and treatment of the COVID-19 disease. The most recent related publications and medical reports were investigated with the purpose of choosing inputs and targets of the network that could facilitate reaching a reliable Artificial Neural Network-based tool for challenges associated with COVID-19. Furthermore, there are some specific inputs for each platform, including various forms of the data, such as clinical data and medical imaging which can improve the performance of the introduced approaches toward the best responses in practical applications.

链接：https://ieeexplore.ieee.org/document/9115663

3.标题：Peeking Inside the Black-Box: A Survey on Explainable Artificial Intelligence (XAI)

出处： IEEE Access

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

4.标题：COVID-19 Artificial Intelligence Diagnosis Using Only Cough Recordings

出处： IEEE Open Journal of Engineering in Medicine and Biology

作者：Jordi Laguarta; Ferran Hueto; Brian Subirana

摘要：Goal: We hypothesized that COVID-19 subjects, especially including asymptomatics, could be accurately discriminated only from a forced-cough cell phone recording using Artificial Intelligence. To train our MIT Open Voice model we built a data collection pipeline of COVID-19 cough recordings through our website (opensigma.mit.edu) between April and May 2020 and created the largest audio COVID-19 cough balanced dataset reported to date with 5,320 subjects. Methods: We developed an AI speech processing framework that leverages acoustic biomarker feature extractors to pre-screen for COVID-19 from cough recordings, and provide a personalized patient saliency map to longitudinally monitor patients in real-time, non-invasively, and at essentially zero variable cost. Cough recordings are transformed with Mel Frequency Cepstral Coefficient and inputted into a Convolutional Neural Network (CNN) based architecture made up of one Poisson biomarker layer and 3 pre-trained ResNet50's in parallel, outputting a binary

pre-screening diagnostic. Our CNN-based models have been trained on 4256 subjects and tested on the remaining 1064 subjects of our dataset. Transfer learning was used to learn biomarker features on larger datasets, previously successfully tested in our Lab on Alzheimer's, which significantly improves the COVID-19 discrimination accuracy of our architecture. Results: When validated with subjects diagnosed using an official test, the model achieves COVID-19 sensitivity of 98.5% with a specificity of 94.2% (AUC: 0.97). For asymptomatic subjects it achieves sensitivity of 100% with a specificity of 83.2%. Conclusions: AI techniques can produce a free, non-invasive, real-time, any-time, instantly distributable, large-scale COVID-19 asymptomatic screening tool to augment current approaches in containing the spread of COVID-19. Practical use cases could be for daily screening of students, workers, and public as schools, jobs, and transport reopen, or for pool testing to quickly alert of outbreaks in groups. General speech biomarkers may exist that cover several disease categories, as we demonstrated using the same ones for COVID-19 and Alzheimer's.

链接：https://ieeexplore.ieee.org/document/9208795

5.标题：SegNet: A Deep Convolutional Encoder-Decoder Architecture for Image Segmentation

出处： IEEE Transactions on Pattern Analysis and Machine Intelligence

作者：Vijay Badrinarayanan; Alex Kendall; Roberto Cipolla

摘要：We present a novel and practical deep fully convolutional neural network architecture for semantic pixel-wise segmentation termed SegNet. This core trainable segmentation engine consists of an encoder network, a corresponding decoder network followed by a pixel-wise classification layer. The architecture of the encoder network is topologically identical to the 13 convolutional layers in the VGG16 network [1] . The role of the decoder network is to map the low resolution encoder feature maps to full input resolution feature maps for pixel-wise classification. The novelty of SegNet lies is in the manner in which the decoder upsamples its lower resolution input feature map(s). Specifically, the decoder uses pooling indices computed in the max-pooling step of the corresponding encoder to perform non-linear upsampling. This eliminates the need for learning to upsample. The upsampled maps are sparse and are then convolved with trainable filters to produce dense feature maps. We compare our proposed architecture with the widely adopted FCN [2] and also with the well known DeepLab-LargeFOV [3] , DeconvNet [4] architectures. This comparison reveals the memory versus accuracy trade-off involved in achieving good segmentation performance. SegNet was primarily motivated by scene understanding applications. Hence, it is designed to be efficient both in terms of memory and computational time during inference. It is also significantly smaller in the number of trainable parameters than other competing architectures and can be trained end-to-end using stochastic gradient descent. We also performed a controlled benchmark of SegNet and other architectures on both road scenes and SUN RGB-D indoor scene segmentation tasks. These quantitative assessments show that SegNet provides good performance with competitive inference time and most efficient inference memory-wise as compared to other architectures. We also provide a Caffe implementation of SegNet and a web demo at http://mi.eng.cam.ac.uk/projects/segnet/.

链接：https://ieeexplore.ieee.org/document/7803544

6.标题：A Comprehensive Review of the COVID-19 Pandemic and the Role of IoT, Drones, AI, Blockchain, and 5G in Managing its Impact

出处： IEEE Access

作者：Vinay Chamola; Vikas Hassija; Vatsal Gupta; Mohsen Guizani

摘要：The unprecedented outbreak of the 2019 novel coronavirus, termed as COVID-19 by the World Health Organization (WHO), has placed numerous governments around the world in a precarious position. The impact of the COVID-19 outbreak, earlier witnessed by the citizens of China alone, has now become a matter of grave concern for virtually every country in the world. The scarcity of resources to endure the COVID-19 outbreak combined with the fear of overburdened healthcare systems has forced a majority of these countries into a state of partial or complete lockdown. The number of laboratory-confirmed coronavirus cases has been increasing at an alarming rate throughout the world, with reportedly more than 3 million confirmed cases as of 30 April 2020. Adding to these woes, numerous false reports, misinformation, and unsolicited fears in regards to coronavirus, are being circulated regularly since the outbreak of the COVID-19. In response to such acts, we draw on various reliable sources to present a detailed review of all the major aspects associated with the COVID-19 pandemic. In addition to the direct health implications associated with the outbreak of COVID-19, this study highlights its impact on the global economy. In drawing things to a close, we explore the use of technologies such as the Internet of Things (IoT), Unmanned Aerial Vehicles (UAVs), blockchain, Artificial Intelligence (AI), and 5G, among others, to help mitigate the impact of COVID-19 outbreak.

链接：https://ieeexplore.ieee.org/document/9086010

7.标题：Internet of Things for Smart Cities

出处：IEEE Internet of Things Journal

作者：Andrea Zanella; Nicola Bui; Angelo Castellani; Lorenzo Vangelista; Michele Zorzi

摘要：The Internet of Things (IoT) shall be able to incorporate transparently and seamlessly a large number of different and heterogeneous end systems, while providing open access to selected subsets of data for the development of a plethora of digital services. Building a general architecture for the IoT is hence a very complex task, mainly because of the extremely large variety of devices, link layer technologies, and services that may be involved in such a system. In this paper, we focus specifically to an urban IoT system that, while still being quite a broad category, are characterized by their specific application domain. Urban IoTs, in fact, are designed to support the Smart City vision, which aims at exploiting the most advanced communication technologies to support added-value services for the administration of the city and for the citizens. This paper hence provides a comprehensive survey of the enabling technologies, protocols, and architecture for an urban IoT. Furthermore, the paper will present and discuss the technical solutions and best-practice guidelines adopted in the Padova Smart City project, a proof-of-concept deployment of an IoT island in the city of Padova, Italy, performed in collaboration with the city municipality.

链接：https://ieeexplore.ieee.org/document/6740844

8.标题： Formulating and Solving Routing Problems on Quantum Computers
出处： IEEE Transactions on Quantum Engineering
作者： Stuart Harwood; Claudio Gambella; Dimitar Trenev; Andrea Simonetto; David Bernal; Donny Greenberg
摘要： The determination of vehicle routes fulfilling connectivity, time, and operational constraints is a well-studied combinatorial optimization problem. The NP-hard complexity of vehicle routing problems has fostered the adoption of tailored exact approaches, matheuristics, and metaheuristics on classical computing devices. The ongoing evolution of quantum computing hardware and the recent advances of quantum algorithms (i.e., VQE, QAOA, and ADMM) for mathematical programming make decision-making for routing problems an avenue of research worthwhile to be explored on quantum devices. In this article, we propose several mathematical formulations for inventory routing cast as vehicle routing with time windows and comment on their strengths and weaknesses. The optimization models are compared from a quantum computing perspective, specifically with metrics to evaluate the difficulty in solving the underlying quadratic unconstrained binary optimization problems. Finally, the solutions obtained on simulated quantum devices demonstrate the relative benefits of different algorithms and their robustness when put into practice.
链接： https://ieeexplore.ieee.org/document/9314905

9.标题： A Comprehensive Survey on Graph Neural Networks
出处： IEEE Transactions on Neural Networks and Learning Systems
作者： Zonghan Wu; Shirui Pan; Fengwen Chen; Guodong Long; Chengqi Zhang; Philip S. Yu
摘要： Deep learning has revolutionized many machine learning tasks in recent years, ranging from image classification and video processing to speech recognition and natural language understanding. The data in these tasks are typically represented in the Euclidean space. However, there is an increasing number of applications, where data are generated from non-Euclidean domains and are represented as graphs with complex relationships and interdependency between objects. The complexity of graph data has imposed significant challenges on the existing machine learning algorithms. Recently, many studies on extending deep learning approaches for graph data have emerged. In this article, we provide a comprehensive overview of graph neural networks (GNNs) in data mining and machine learning fields. We propose a new taxonomy to divide the state-of-the-art GNNs into four categories, namely, recurrent GNNs, convolutional GNNs, graph autoencoders, and spatial-temporal GNNs. We further discuss the applications of GNNs across various domains and summarize the open-source codes, benchmark data sets, and model evaluation of GNNs. Finally, we propose potential research directions in this rapidly growing field.
链接： https://ieeexplore.ieee.org/document/9046288

10.标题： Drone-Based Material Transfer System in a Robotic Mobile Fulfillment Center
出处： IEEE Transactions on Automation Science and Engineering
作者： Andy Ham
摘要： Deploying unmanned aerial vehicles, also known as drones, for final-mile delivery in logistics operations has inspired this research. One conceivable scenario is to use the drone to

transfer jobs in a robotic mobile fulfillment center. Each job might be characterized by origin, destination, time window, and precedence relation. In particular, a take-away conveyor is continuously pushing forward shipping cartons, wherein drones must pick up jobs and drop them off to the cartons within the time window since the cartons would be closed and labeled at the end of the conveyor. Furthermore, each job contains two subtransfers for drone: flight from drone's current location to pickup location and flight to dropoff location. Two exact approaches are proposed-a mixed integer programming and a constraint programming-and tested for a real-time perspective.

链接：https://ieeexplore.ieee.org/document/8920130

11.标题：Deep Residual Learning for Image Recognition

出处：2016 IEEE Conference on Computer Vision and Pattern Recognition

作者：Kaiming He; Xiangyu Zhang; Shaoqing Ren; Jian Sun

摘要：Deeper neural networks are more difficult to train. We present a residual learning framework to ease the training of networks that are substantially deeper than those used previously. We explicitly reformulate the layers as learning residual functions with reference to the layer inputs, instead of learning unreferenced functions. We provide comprehensive empirical evidence showing that these residual networks are easier to optimize, and can gain accuracy from considerably increased depth. On the ImageNet dataset we evaluate residual nets with a depth of up to 152 layers - 8× deeper than VGG nets [40] but still having lower complexity. An ensemble of these residual nets achieves 3.57% error on the ImageNet test set. This result won the 1st place on the ILSVRC 2015 classification task. We also present analysis on CIFAR-10 with 100 and 1000 layers. The depth of representations is of central importance for many visual recognition tasks. Solely due to our extremely deep representations, we obtain a 28% relative improvement on the COCO object detection dataset. Deep residual nets are foundations of our submissions to ILSVRC & COCO 2015 competitions1, where we also won the 1st places on the tasks of ImageNet detection, ImageNet localization, COCO detection, and COCO segmentation.

链接：https://ieeexplore.ieee.org/document/7780459

12.标题：A Survey of Data Mining and Machine Learning Methods for Cyber Security Intrusion Detection

出处：IEEE Communications Surveys & Tutorials

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

13.标题：A Survey of 5G Network: Architecture and Emerging Technologies
出处： IEEE Access
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

14.标题：Machine Learning and Deep Learning Methods for Cybersecurity
出处： IEEE Access
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

15.标题：Effective Heart Disease Prediction Using Hybrid Machine Learning Techniques
出处： IEEE Access
作者：Senthilkumar Mohan; Chandrasegar Thirumalai; Gautam Srivastava
摘要：Heart disease is one of the most significant causes of mortality in the world today. Prediction of cardiovascular disease is a critical challenge in the area of clinical data analysis. Machine learning (ML) has been shown to be effective in assisting in making decisions and predictions from the large quantity of data produced by the healthcare industry. We have also seen ML techniques being used in recent developments in different areas of the Internet of Things (IoT).

Various studies give only a glimpse into predicting heart disease with ML techniques. In this paper, we propose a novel method that aims at finding significant features by applying machine learning techniques resulting in improving the accuracy in the prediction of cardiovascular disease. The prediction model is introduced with different combinations of features and several known classification techniques. We produce an enhanced performance level with an accuracy level of 88.7% through the prediction model for heart disease with the hybrid random forest with a linear model (HRFLM).

链接：https://ieeexplore.ieee.org/document/8740989

16.标题：6G Wireless Communication Systems: Applications, Requirements, Technologies, Challenges, and Research Directions

出处： IEEE Open Journal of the Communications Society

作者：Mostafa Zaman Chowdhury; Md. Shahjalal; Shakil Ahmed; Yeong Min Jang

摘要：The demand for wireless connectivity has grown exponentially over the last few decades. Fifth-generation (5G) communications, with far more features than fourth-generation communications, will soon be deployed worldwide. A new paradigm of wireless communication, the sixth-generation (6G) system, with the full support of artificial intelligence, is expected to be implemented between 2027 and 2030. Beyond 5G, some fundamental issues that need to be addressed are higher system capacity, higher data rate, lower latency, higher security, and improved quality of service (QoS) compared to the 5G system. This paper presents the vision of future 6G wireless communication and its network architecture. This article describes emerging technologies such as artificial intelligence, terahertz communications, wireless optical technology, free-space optical network, blockchain, three-dimensional networking, quantum communications, unmanned aerial vehicles, cell-free communications, integration of wireless information and energy transfer, integrated sensing and communication, integrated access-backhaul networks, dynamic network slicing, holographic beamforming, backscatter communication, intelligent reflecting surface, proactive caching, and big data analytics that can assist the 6G architecture development in guaranteeing the QoS. Besides, expected applications with 6G communication requirements and possible technologies are presented. We also describe potential challenges and research directions for achieving this goal.

链接：https://ieeexplore.ieee.org/document/9144301

17.标题：Edge Intelligence: Paving the Last Mile of Artificial Intelligence With Edge Computing

出处： Proceedings of the IEEE

作者：Zhi Zhou; Xu Chen; En Li; Liekang Zeng; Ke Luo; Junshan Zhang

摘要：With the breakthroughs in deep learning, the recent years have witnessed a booming of artificial intelligence (AI) applications and services, spanning from personal assistant to recommendation systems to video/audio surveillance. More recently, with the proliferation of mobile computing and Internet of Things (IoT), billions of mobile and IoT devices are connected to the Internet, generating zillions bytes of data at the network edge. Driving by this trend, there is an urgent need to push the AI frontiers to the network edge so as to fully unleash the potential of the edge big data. To meet this demand, edge computing, an emerging paradigm that pushes computing tasks and services from the network core to the network edge, has been widely

recognized as a promising solution. The resulted new interdiscipline, edge AI or edge intelligence (EI), is beginning to receive a tremendous amount of interest. However, research on EI is still in its infancy stage, and a dedicated venue for exchanging the recent advances of EI is highly desired by both the computer system and AI communities. To this end, we conduct a comprehensive survey of the recent research efforts on EI. Specifically, we first review the background and motivation for AI running at the network edge. We then provide an overview of the overarching architectures, frameworks, and emerging key technologies for deep learning model toward training/inference at the network edge. Finally, we discuss future research opportunities on EI. We believe that this survey will elicit escalating attentions, stimulate fruitful discussions, and inspire further research ideas on EI.

链接：https://ieeexplore.ieee.org/document/8736011

18.标题：Review of Deep Learning Algorithms and Architectures

出处： IEEE Access

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

19.标题：Unmanned Aerial Vehicles (UAVs): A Survey on Civil Applications and Key Research Challenges

出处： IEEE Access

作者：Hazim Shakhatreh;Ahmad H. Sawalmeh;Ala Al-Fuqaha;Zuochao Dou;Eyad Almaita;Issa Khalil;Noor Shamsiah Othman;Abdallah Khreishah;Mohsen Guizani

摘要：The use of unmanned aerial vehicles (UAVs) is growing rapidly across many civil application domains, including real-time monitoring, providing wireless coverage, remote sensing, search and rescue, delivery of goods, security and surveillance, precision agriculture, and civil infrastructure inspection. Smart UAVs are the next big revolution in the UAV technology promising to provide new opportunities in different applications, especially in civil infrastructure in terms of reduced risks and lower cost. Civil infrastructure is expected to dominate more than $45 Billion market value of UAV usage. In this paper, we present UAV civil applications and their challenges. We also discuss the current research trends and provide future insights for potential

UAV uses. Furthermore, we present the key challenges for UAV civil applications, including charging challenges, collision avoidance and swarming challenges, and networking and security-related challenges. Based on our review of the recent literature, we discuss open research challenges and draw high-level insights on how these challenges might be approached.
链接：https://ieeexplore.ieee.org/document/8682048

20.标题：Intelligent Reflecting Surface-Enhanced OFDM: Channel Estimation and Reflection Optimization
出处： IEEE Wireless Communications Letters
作者：Beixiong Zheng; Rui Zhang
摘要：In the intelligent reflecting surface (IRS)-enhanced wireless communication system, channel state information (CSI) is of paramount importance for achieving the passive beamforming gain of IRS, which, however, is a practically challenging task due to its massive number of passive elements without transmitting/receiving capabilities. In this letter, we propose a practical transmission protocol to execute channel estimation and reflection optimization successively for an IRS-enhanced orthogonal frequency division multiplexing (OFDM) system. Under the unit-modulus constraint, a novel reflection pattern at the IRS is designed to aid the channel estimation at the access point (AP) based on the received pilot signals from the user, for which the channel estimation error is derived in closed-form. With the estimated CSI, the reflection coefficients are then optimized by a low-complexity algorithm based on the resolved strongest signal path in the time domain. Simulation results corroborate the effectiveness of the proposed channel estimation and reflection optimization methods.
链接：https://ieeexplore.ieee.org/document/8937491

21.标题：An Airborne Sonar System for Underwater Remote Sensing and Imaging
出处：IEEE Access
作者：Aidan Fitzpatrick; Ajay Singhvi; Amin Arbabian
摘要：High-resolution imaging and mapping of the ocean and its floor has been limited to less than 5% of the global waters due to technological barriers. Whereas sonar is the primary contributor to existing underwater imagery, the water-based system is limited in spatial coverage due to its low imaging throughput. On the other hand, aerial synthetic aperture radar systems have provided high-resolution imaging of the entire earth's landscapes but are incapable of deep penetration into water. In this work, we present a proof-of-concept system which bridges the gap between electromagnetic imaging in air and sonar imaging in water through the laser-induced photoacoustic effect and high-sensitivity airborne ultrasonic detection. Here, we use air-coupled capacitive micromachined ultrasonic transducers (CMUTs) which is a critical differentiator from previous works and has enabled the acquisition of an underwater image from a fully airborne acoustic imaging system - a task that has yet to be accomplished in the literature. With the entire imaging system located on an airborne platform, there is much promise for the scalability of our system to one which could perform high-throughput imaging of underwater in large-scale deployment. Non-contact acoustic-based imaging modalities are also of much interest to the medical imaging and non-destructive testing communities. Incorporating air-coupled transducers, for example CMUTs, or other resonant sensors in these applications could be aided by the analysis

presented throughout this work.

链接：https://ieeexplore.ieee.org/document/9228880

22.标题：The Graph Neural Network Model

出处： IEEE Transactions on Neural Networks

作者：Franco Scarselli;Marco Gori;Ah Chung Tsoi;Markus Hagenbuchner;Gabriele Monfardini

摘要：Many underlying relationships among data in several areas of science and engineering, e.g., computer vision, molecular chemistry, molecular biology, pattern recognition, and data mining, can be represented in terms of graphs. In this paper, we propose a new neural network model, called graph neural network (GNN) model, that extends existing neural network methods for processing the data represented in graph domains. This GNN model, which can directly process most of the practically useful types of graphs, e.g., acyclic, cyclic, directed, and undirected, implements a function tau(G,n) isin IR m that maps a graph G and one of its nodes n into an m -dimensional Euclidean space. A supervised learning algorithm is derived to estimate the parameters of the proposed GNN model. The computational cost of the proposed algorithm is also considered. Some experimental results are shown to validate the proposed learning algorithm, and to demonstrate its generalization capabilities.

链接：https://ieeexplore.ieee.org/document/4700287

23.标题：Change Management Models: A Comparative Analysis and Concerns

出处： IEEE Engineering Management Review

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

24.标题：Can AI Help in Screening Viral and COVID-19 Pneumonia?

出处： IEEE Access

作者：Muhammad E. H. Chowdhury;Tawsifur Rahman;Amith Khandakar;Rashid Mazhar;Muhammad Abdul Kadir;Zaid Bin Mahbub;Khandakar Reajul Islam;Muhammad Salman Khan;Atif Iqbal;Nasser Al Emadi;Mamun Bin Ibne Reaz;Mohammad Tariqul Islam

摘要：Coronavirus disease (COVID-19) is a pandemic disease, which has already caused thousands of causalities and infected several millions of people worldwide. Any technological tool enabling rapid screening of the COVID-19 infection with high accuracy can be crucially helpful to the healthcare professionals. The main clinical tool currently in use for the diagnosis of COVID-19 is the Reverse transcription polymerase chain reaction (RT-PCR), which is expensive, less-sensitive and requires specialized medical personnel. X-ray imaging is an easily accessible tool that can be an excellent alternative in the COVID-19 diagnosis. This research was taken to investigate the utility of artificial intelligence (AI) in the rapid and accurate detection of COVID-19 from chest X-ray images. The aim of this paper is to propose a robust technique for automatic detection of COVID-19 pneumonia from digital chest X-ray images applying

pre-trained deep-learning algorithms while maximizing the detection accuracy. A public database was created by the authors combining several public databases and also by collecting images from recently published articles. The database contains a mixture of 423 COVID-19, 1485 viral pneumonia, and 1579 normal chest X-ray images. Transfer learning technique was used with the help of image augmentation to train and validate several pre-trained deep Convolutional Neural Networks (CNNs). The networks were trained to classify two different schemes: i) normal and COVID-19 pneumonia; ii) normal, viral and COVID-19 pneumonia with and without image augmentation. The classification accuracy, precision, sensitivity, and specificity for both the schemes were 99.7%, 99.7%, 99.7% and 99.55% and 97.9%, 97.95%, 97.9%, and 98.8%, respectively. The high accuracy of this computer-aided diagnostic tool can significantly improve the speed and accuracy of COVID-19 diagnosis. This would be extremely useful in this pandemic where disease burden and need for preventive measures are at odds with available resources.

链接：https://ieeexplore.ieee.org/document/9144185

25.标题：DeepAnT: A Deep Learning Approach for Unsupervised Anomaly Detection in Time Series

出处： IEEE Access

作者：Mohsin Munir; Shoaib Ahmed Siddiqui; Andreas Dengel; Sheraz Ahmed

摘要：Traditional distance and density-based anomaly detection techniques are unable to detect periodic and seasonality related point anomalies which occur commonly in streaming data, leaving a big gap in time series anomaly detection in the current era of the IoT. To address this problem, we present a novel deep learning-based anomaly detection approach (DeepAnT) for time series data, which is equally applicable to the non-streaming cases. DeepAnT is capable of detecting a wide range of anomalies, i.e., point anomalies, contextual anomalies, and discords in time series data. In contrast to the anomaly detection methods where anomalies are learned, DeepAnT uses unlabeled data to capture and learn the data distribution that is used to forecast the normal behavior of a time series. DeepAnT consists of two modules: time series predictor and anomaly detector. The time series predictor module uses deep convolutional neural network (CNN) to predict the next time stamp on the defined horizon. This module takes a window of time series (used as a context) and attempts to predict the next time stamp. The predicted value is then passed to the anomaly detector module, which is responsible for tagging the corresponding time stamp as normal or abnormal. DeepAnT can be trained even without removing the anomalies from the given data set. Generally, in deep learning-based approaches, a lot of data are required to train a model. Whereas in DeepAnT, a model can be trained on relatively small data set while achieving good generalization capabilities due to the effective parameter sharing of the CNN. As the anomaly detection in DeepAnT is unsupervised, it does not rely on anomaly labels at the time of model generation. Therefore, this approach can be directly applied to real-life scenarios where it is practically impossible to label a big stream of data coming from heterogeneous sensors comprising of both normal as well as anomalous points. We have performed a detailed evaluation of 15 algorithms on 10 anomaly detection benchmarks, which contain a total of 433 real and synthetic time series. Experiments show that DeepAnT outperforms the state-of-the-art anomaly detection methods in most of the cases, while performing on par with others.

链接：https://ieeexplore.ieee.org/document/8581424

ESI HOT PAPERS

(Chemistry)

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

1.被引频次：624

题目：EFFICIENT, STABLE AND SCALABLE PEROVSKITE SOLAR CELLS USING POLY(3-HEXYLTHIOPHENE)

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出处：NATURE 567 (7749): 511-+ MAR 28 2019

摘要： Perovskite solar cells typically comprise electron-and hole-transport materials deposited on each side of a perovskite active layer. So far, only two organic hole-transport materials have led to state-of-the-art performance in these solar cells(1): poly(triarylamine) (PTAA)(2-5) and 2,2',7,7'-tetrakis(N,N-di-p-methoxyphenylamine)-9,9'-spirobifluorene (spiro-OMeTAD)(6,7). However, these materials have several drawbacks in terms of commercialization, including high cost(8), the need for hygroscopic dopants that trigger degradation of the perovskite layer(9) and limitations in their deposition processes(10). Poly(3-hexylthiophene) (P3HT) is an alternative hole-transport material with excellent optoelectronic properties(11-13), low cost(8,14) and ease of fabrication(15-18), but so far the efficiencies of perovskite solar cells using P3HT have reached only around 16 per cent(19). Here we propose a device architecture for highly efficient perovskite solar cells that use P3HT as a hole-transport material without any dopants. A thin layer of wide-bandgap halide perovskite is formed on top of the narrow-bandgap light-absorbing layer by an in situ reaction of n-hexyl trimethyl ammonium bromide on the perovskite surface. Our device has a certified power conversion efficiency of 22.7 per cent with hysteresis of +/- 0.51 per cent; exhibits good stability at 85 per cent relative humidity without encapsulation; and upon encapsulation demonstrates long-term operational stability for 1,370 hours under 1-Sun illumination at room temperature, maintaining 95 per cent of the initial efficiency. We extend our platform to large-area modules (24.97 square centimetres)-which are fabricated using a scalable bar-coating method for the deposition of P3HT-and achieve a power conversion efficiency of 16.0 per cent. Realizing the potential of P3HT as a hole-transport material by using a wide-bandgap halide could be a valuable direction for perovskite solar-cell research.

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2.被引频次：539

题目：ACHIEVING OVER 16% EFFICIENCY FOR SINGLE-JUNCTION ORGANIC SOLAR CELLS

作者：FAN, BB;ZHANG, DF;LI, MJ;ZHONG, WK;ZENG, ZMY;YING, L;HUANG, F;CAO, Y 出处：SCIENCE CHINA-CHEMISTRY 62 (6): 746-752 JUN 2019

摘要：To achieve high photovoltaic performance of bulk hetero-junction organic solar cells (OSCs), a range of critical factors including absorption profiles, energy level alignment, charge carrier mobility and miscibility of donor and acceptor materials should be carefully considered. For electron-donating materials, the deep highest occupied molecular orbital (HOMO) energy level that is beneficial for high open-circuit voltage is much appreciated. However, a new issue in charge transfer emerges when matching such a donor with an acceptor that has a shallower HOMO energy level. More to this point, the chemical strategies used to enhance the absorption coefficient of acceptors may lead to increased molecular crystallinity, and thus result in less controllable phase-separation of photoactive layer. Therefore, to realize balanced photovoltaic parameters, the donor-acceptor combinations should simultaneously address the absorption spectra, energy levels, and film morphologies. Here, we selected two non-fullerene acceptors, namely BTPT-4F and BTPTT-4F, to match with a wide-bandgap polymer donor P2F-EHp consisting of an imide-functionalized benzotriazole moiety, as these materials presented complementary absorption and well-matched energy levels. By delicately optimizing the blend film morphology, we demonstrated an unprecedented power conversion efficiency of over 16% for the device based on P2F-EHp:BTPTT-4F, suggesting the great promise of materials matching toward high-performance OSCs.

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3.被引频次：525

题目：NANOMATERIALS WITH ENZYME-LIKE CHARACTERISTICS (NANOZYMES): NEXT-GENERATION ARTIFICIAL ENZYMES (II)

作者：WU, JJX;WANG, XY;WANG, Q;LOU, ZP;LI, SR;ZHU, YY;QIN, L;WEI, H

出处：CHEMICAL SOCIETY REVIEWS 48 (4): 1004-1076 FEB 21 201

摘要：Nanozymes are nanomaterials with enzyme-like characteristics (Chem. Soc. Rev., 2013, 42, 6060-6093). They have been developed to address the limitations of natural enzymes and conventional artificial enzymes. Along with the significant advances in nanotechnology, biotechnology, catalysis science, and computational design, great progress has been achieved in the field of nanozymes since the publication of the above-mentioned comprehensive review in 2013. To highlight these achievements, this review first discusses the types of nanozymes and their representative nanomaterials, together with the corresponding catalytic mechanisms whenever available. Then, it summarizes various strategies for modulating the activity and selectivity of nanozymes. After that, the broad applications from biomedical analysis and imaging to theranostics and environmental protection are covered. Finally, the current challenges faced by nanozymes are outlined and the future directions for advancing nanozyme research are suggested.

The current review can help researchers know well the current status of nanozymes and may catalyze breakthroughs in this field.

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4.被引频次：509

题目：3D TRANSITION METALS FOR C-H ACTIVATION

作者：GANDEEPAN, P;MULLER, T;ZELL, D;CERA, G;WARRATZ, S;ACKERMANN, L

出处：CHEMICAL REVIEWS 119 (4): 2192-2452 SP. ISS. SI FEB 27 2019

摘要：C-H activation has surfaced as an increasingly powerful tool for molecular sciences, with notable applications to material sciences, crop protection, drug discovery, and pharmaceutical industries, among others. Despite major advances, the vast majority of these C-H functionalizations required precious 4d or 5d transition metal catalysts. Given the cost-effective and sustainable nature of earth-abundant first row transition metals, the development of less toxic, inexpensive 3d metal catalysts for C-H activation has gained considerable recent momentum as a significantly more environmentally-benign and economically-attractive alternative. Herein, we provide a comprehensive overview on first row transition metal catalysts for C-H activation until summer 2018.

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5.被引频次：443

题目：PHOTOTHERMAL THERAPY AND PHOTOACOUSTIC IMAGING VIA NANOTHERANOSTICS IN FIGHTING CANCER

作者：LIU, YJ;BHATTARAI, P;DAI, ZF;CHEN, XY

出处：CHEMICAL SOCIETY REVIEWS 48 (7): 2053-2108 APR 7 2019

摘要：The nonradiative conversion of light energy into heat (photothermal therapy, PTT) or sound energy (photoacoustic imaging, PAI) has been intensively investigated for the treatment and diagnosis of cancer, respectively. By taking advantage of nanocarriers, both imaging and therapeutic functions together with enhanced tumour accumulation have been thoroughly studied to improve the pre-clinical efficiency of PAI and PTT. In this review, we first summarize the development of inorganic and organic nano photothermal transduction agents (PTAs) and strategies for improving the PTT outcomes, including applying appropriate laser dosage, guiding the treatment via imaging techniques, developing PTAs with absorption in the second NIR window, increasing photothermal conversion efficiency (PCE), and also increasing the accumulation of PTAs in tumours. Second, we introduce the advantages of combining PTT with other therapies in cancer treatment. Third, the emerging applications of PAI in cancer-related

research are exemplified. Finally, the perspectives and challenges of PTT and PAI for combating cancer, especially regarding their clinical translation, are discussed. We believe that PTT and PAI having noteworthy features would become promising next-generation non-invasive cancer theranostic techniques and improve our ability to combat cancers.

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6.被引频次：430

题目：ULTRATHIN 2D/2D WO3/G-C3N4 STEP-SCHEME H-2-PRODUCTION PHOTOCATALYST

作者：FU, JW;XU, QL;LOW, JX;JIANG, CJ;YU, JG

出处：APPLIED CATALYSIS B-ENVIRONMENTAL 243: 556-565 APR 2019

摘要：The appropriate interfacial contact of heterojunction photocatalysts plays a critical role in transfer/separation of interfacial charge carriers. Design of two-dimensional (2D)/2D surface-to-surface heterojunction is an effective method for improving photocatalytic activity since greater contact area can enhance interfacial charge transfer rate. Herein, ultrathin 2D/2D WO3/g-C3N4 step-like composite heterojunction photocatalysts were fabricated by electrostatic self-assembly of ultrathin tungsten trioxide (WO3) and graphitic carbon nitride (g-C3N4) nanosheets. The ultrathin WO3 and g-C3N4 nanosheets were obtained by electrostatic-assisted ultrasonic exfoliation of bulk WO3 and a two-step thermal-etching of bulk g-C3N4, respectively. The thickness of ultrathin WO3 and g-C3N4 nanosheets are 2.5-3.5 nm, which is equivalent to 5-8 atomic or molecular layer thickness. This ultrathin layered heterojunction structure can enhance surface photocatalytic rate because photogenerated electrons and holes at heterogeneous interface more easily transfer to surface of photocatalysts. Therefore, the obtained ultrathin 2D/2D WO3/g-C3N4 step-scheme (S-scheme) heterojunction photocatalysts exhibited better Hz-production activity than pure g-C3N4 and WO3 with the same loading amount of Pt as cocatalyst. The mechanism and driving force of charge transfer and separation in S-scheme heterojunction photocatalysts are investigated and discussed. This investigation will provide new insight about designing and constructing novel S-scheme heterojunction photocatalysts.

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7.被引频次：428

题目：NANOPARTICLES: PROPERTIES, APPLICATIONS AND TOXICITIES

作者：KHAN, I;SAEED, K;KHAN, I

出处：ARABIAN JOURNAL OF CHEMISTRY 12 (7): 908-931 NOV 2019

摘要：This review is provided a detailed overview of the synthesis, properties and applications of

nanoparticles (NPs) exist in different forms. NPs are tiny materials having size ranges from 1 to 100 nm. They can be classified into different classes based on their properties, shapes or sizes. The different groups include fullerenes, metal NPs, ceramic NPs, and polymeric NPs. NPs possess unique physical and chemical properties due to their high surface area and nanoscale size. Their optical properties are reported to be dependent on the size, which imparts different colors due to absorption in the visible region. Their reactivity, toughness and other properties are also dependent on their unique size, shape and structure. Due to these characteristics, they are suitable candidates for various commercial and domestic applications, which include catalysis, imaging, medical applications, energy-based research, and environmental applications. Heavy metal NPs of lead, mercury and tin are reported to be so rigid and stable that their degradation is not easily achievable, which can lead to many environmental toxicities. (C) 2017 The Authors. Production and hosting by Elsevier B.V.

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8.被引频次：414
题目：HALIDE PEROVSKITE PHOTOVOLTAICS: BACKGROUND, STATUS, AND FUTURE PROSPECTS
作者：JENA, AK;KULKARNI, A;MIYASAKA, T
出处：CHEMICAL REVIEWS 119 (5): 3036-3103 SP. ISS. SI MAR 13 2019
摘要：The photovoltaics of organic inorganic lead halide perovskite materials have shown rapid improvements in solar cell performance, surpassing the top efficiency of semiconductor compounds such as CdTe and CIGS (copper indium gallium selenide) used in solar cells in just about a decade. Perovskite preparation via simple and inexpensive solution processes demonstrates the immense potential of this thin-film solar cell technology to become a low-cost alternative to the presently commercially available photovoltaic technologies. Significant developments in almost all aspects of perovskite solar cells and discoveries of some fascinating properties of such hybrid perovskites have been made recently. This Review describes the fundamentals, recent research progress, present status, and our views on future prospects of perovskite-based photovoltaics, with discussions focused on strategies to improve both intrinsic and extrinsic (environmental) stabilities of high-efficiency devices. Strategies and challenges regarding compositional engineering of the hybrid perovskite structure are discussed, including potentials for developing all-inorganic and lead-free perovskite materials. Looking at the latest cutting-edge research, the prospects for perovskite-based photovoltaic and optoelectronic devices, including non-photovoltaic applications such as X-ray detectors and image sensing devices in industrialization, are described. In addition to the aforementioned major topics, we also review, as a background, our encounter with perovskite materials for the first solar cell application, which should inspire young researchers in chemistry and physics to identify and work on challenging interdisciplinary research problems through exchanges between academia and industry.
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9.被引频次：406
题 目：RECENT DEVELOPMENTS IN HETEROGENEOUS PHOTOCATALYSTS FOR SOLAR-DRIVEN OVERALL WATER SPLITTING
作者：WANG, Z;LI, C;DOMEN, K
出处：CHEMICAL SOCIETY REVIEWS 48 (7): 2109-2125 APR 7 2019
摘要：Overall water splitting based on particulate photocatalysts is an easily constructed and cost-effective technology for the conversion of abundant solar energy into clean and renewable hydrogen energy on a large scale. This promising technology can be achieved in a one-step excitation system using a single photocatalyst or via a Z-scheme process based on a pair of photocatalysts. Ideally, such photocatalysis will proceed with charge separation and transport unaffected by recombination and trapping, and surface catalytic processes will not involve undesirable reactions. This review summarizes the basics of overall water splitting via both one-step excitation and Z-scheme processes, with a focus on standard methods of determining photocatalytic performance. Various surface engineering strategies applied to photocatalysts, such as cocatalyst loading, surface morphology control, surface modification and surface phase junctions, have been developed to allow efficient one-step excitation overall water splitting. In addition, numerous visible-light-responsive photocatalysts have been successfully utilized as H-2-evolution or O-2-evolution photocatalysts in Z-scheme overall water splitting. Prototype particulate immobilization systems with photocatalytic performances comparable to or drastically higher than those of particle suspension systems suggest the exciting possibility of the large-scale production of low-cost renewable solar hydrogen.
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10.被引频次：389
题目：ELECTROSPINNING AND ELECTROSPUN NANOFIBERS: METHODS, MATERIALS, AND APPLICATIONS
作者：XUE, JJ;WU, T;DAI, YQ;XIA, YN
出处：CHEMICAL REVIEWS 119 (8): 5298-5415 APR 24 2019
摘要：Electrospinning is a versatile and viable technique for generating ultrathin fibers. Remarkable progress has been made with regard to the development of electrospinning methods and engineering of electrospun nanofibers to suit or enable various applications. We aim to provide a comprehensive overview of electrospinning, including the principle, methods, materials, and applications. We begin with a brief introduction to the early history of electrospinning, followed by discussion of its principle and typical apparatus. We then discuss its renaissance over

the past two decades as a powerful technology for the production of nanofibers with diversified compositions, structures, and properties. Afterward, we discuss the applications of electrospun nanofibers, including their use as smart mats, filtration membranes, catalytic supports, energy harvesting/conversion/storage components, and photonic and electronic devices, as well as biomedical scaffolds. We highlight the most relevant and recent advances related to the applications of electrospun nanofibers by focusing on the most representative examples. We also offer perspectives on the challenges, opportunities, and new directions for future development. At the end, we discuss approaches to the scale-up production of electrospun nanofibers and briefly discuss various types of commercial products based on electrospun nanofibers that have found widespread use in our everyday life.

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11.被引频次：378

题目：COCATALYSTS FOR SELECTIVE PHOTOREDUCTION OF CO2 INTO SOLAR FUELS

作者：LI, X;YU, JG;JARONIEC, M;CHEN, XB

出处：CHEMICAL REVIEWS 119 (6): 3962-4179 MAR 27 2019

摘要：Photoreduction of CO2 into sustainable and green solar fuels is generally believed to be an appealing solution to simultaneously overcome both environmental problems and energy crisis. The low selectivity of challenging multi-electron CO2 photoreduction reactions makes it one of the holy grails in heterogeneous photocatalysis. This Review highlights the important roles of cocatalysts in selective photocatalytic CO2 reduction into solar fuels using semiconductor catalysts. A special emphasis in this review is placed on the key role, design considerations and modification strategies of cocatalysts for CO2 photoreduction. Various cocatalysts, such as the biomimetic, metal-based, metal-free, and multifunctional ones, and their selectivity for CO2 photoreduction are summarized and discussed, along with the recent advances in this area. This Review provides useful information for the design of highly selective cocatalysts for photo(electro)reduction and electroreduction of CO2 and complements the existing reviews on various semiconductor photocatalysts.

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12.被引频次：345

题目：APPLICATIONS OF 2D MXENES IN ENERGY CONVERSION AND STORAGE SYSTEMS

作者：PANG, JB;MENDES, RG;BACHMATIUK, A;ZHAO, L;TA, HQ;GEMMING, T;LIU, H;LIU, ZF;RUMMELI, MH 出处： CHEMICAL SOCIETY REVIEWS 48 (1): 72-133 JAN 7 2019

摘要：Transition metal carbides and nitrides (MXenes), a family of two-dimensional (2D) inorganic compounds, are materials composed of a few atomic layers of transition metal carbides, nitrides, or carbonitrides. Ti3C2, the first 2D layered MXene, was isolated in 2011. This material, which is a layered bulk material analogous to graphite, was derived from its 3D phase, Ti3AlC2 MAX. Since then, material scientists have either determined or predicted the stable phases of >200 different MXenes based on combinations of various transition metals such as Ti, Mo, V, Cr, and their alloys with C and N. Extensive experimental and theoretical studies have shown their exciting potential for energy conversion and electrochemical storage. To this end, we comprehensively summarize the current advances in MXene research. We begin by reviewing the structure types and morphologies and their fabrication routes. The review then discusses the mechanical, electrical, optical, and electrochemical properties of MXenes. The focus then turns to their exciting potential in energy storage and conversion. Energy storage applications include electrodes in rechargeable lithium-and sodium-ion batteries, lithium-sulfur batteries, and supercapacitors. In terms of energy conversion, photocatalytic fuel production, such as hydrogen evolution from water splitting, and carbon dioxide reduction are presented. The potential of MXenes for the photocatalytic degradation of organic pollutants in water, such as dye waste, is also addressed, along with their promise as catalysts for ammonium synthesis from nitrogen. Finally, their application potential is summarized.

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13.被引频次：333

题目：THE ROLE OF HYDROGEN AND FUEL CELLS IN THE GLOBAL ENERGY SYSTEM

作者：STAFFELL, I;SCAMMAN, D;ABAD, AV;BALCOMBE, P;DODDS, PE;EKINS, P;SHAH, N;WARD, KR

出处：ENERGY & ENVIRONMENTAL SCIENCE 12 (2): 463-491 FEB 1 2019

摘要：Hydrogen technologies have experienced cycles of excessive expectations followed by disillusion. Nonetheless, a growing body of evidence suggests these technologies form an attractive option for the deep decarbonisation of global energy systems, and that recent improvements in their cost and performance point towards economic viability as well. This paper is a comprehensive review of the potential role that hydrogen could play in the provision of electricity, heat, industry, transport and energy storage in a low-carbon energy system, and an assessment of the status of hydrogen in being able to fulfil that potential. The picture that emerges is one of qualified promise: hydrogen is well established in certain niches such as forklift trucks, while mainstream applications are now forthcoming. Hydrogen vehicles are available commercially in several countries, and 225000 fuel cell home heating systems have been sold. This represents a step change from the situation of only five years ago. This review shows that challenges around cost and performance remain, and considerable improvements are still required for hydrogen to become truly competitive. But such competitiveness in the medium-term future no longer seems an unrealistic prospect, which fully justifies the growing interest and policy support for these technologies around the world.

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14.被引频次：333

题目：NANOZYMES: CLASSIFICATION, CATALYTIC MECHANISMS, ACTIVITY REGULATION, AND APPLICATIONS

作者：HUANG, YY;REN, JS;QU, XG

出处：CHEMICAL REVIEWS 119 (6): 4357-4412 MAR 27 2019

摘要：Because of the high catalytic activities and substrate specificity, natural enzymes have been widely used in industrial, medical, and biological fields, etc. Although promising, they often suffer from intrinsic shortcomings such as high cost, low operational stability, and difficulties of recycling. To overcome these shortcomings, researchers have been devoted to the exploration of artificial enzyme mimics for a long time. Since the discovery of ferromagnetic nanoparticles with intrinsic horseradish peroxidase-like activity in 2007, a large amount of studies on nanozymes have been constantly emerging in the next decade. Nanozymes are one kind of nanomaterials with enzymatic catalytic properties. Compared with natural enzymes, nanozymes have the advantages such as low cost, high stability and durability, which have been widely used in industrial, medical, and biological fields. A thorough understanding of the possible catalytic mechanisms will contribute to the development of novel and high-efficient nanozymes, and the rational regulations of the activities of nanozymes are of great significance. In this review, we systematically introduce the classification, catalytic mechanism, activity regulation as well as recent research progress of nanozymes in the field of biosensing, environmental protection, and disease treatments, etc. in the past years. We also propose the current challenges of nanozymes as well as their future research

focus. We anticipate this review may be of significance for the field to understand the properties of nanozymes and the development of novel nanomaterials with enzyme mimicking activities.

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15.被引频次：326

题目：CRITICAL REVIEW OF THE MOLECULAR DESIGN PROGRESS IN NON-FULLERENE ELECTRON ACCEPTORS TOWARDS COMMERCIALLY VIABLE ORGANIC SOLAR CELLS

作者：WADSWORTH, A;MOSER, M;MARKS, A;LITTLE, MS;GASPARINI, N;BRABEC, CJ;BARAN, D;MCCULLOCH, I 出处：CHEMICAL SOCIETY REVIEWS 48 (6): 1596-1625 MAR 21 2019

摘要：Fullerenes have formed an integral part of high performance organic solar cells over the last 20 years, however their inherent limitations in terms of synthetic flexibility, cost and stability have acted as a motivation to develop replacements; the so-called non-fullerene electron acceptors. A rapid evolution of such materials has taken place over the last few years, yielding a number of promising candidates that can exceed the device performance of fullerenes and provide opportunities to improve upon the stability and processability of organic solar cells. In this review we explore the structure-property relationships of a library of non-fullerene acceptors, highlighting the important chemical modifications that have led to progress in the field and provide an outlook for future innovations in electron acceptors for use in organic photovoltaics.

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16.被引频次：322

题目：DEVELOPMENT OF ORGANIC SEMICONDUCTING MATERIALS FOR DEEP-TISSUE OPTICAL IMAGING, PHOTOTHERAPY AND PHOTOACTIVATION

作者：LI, JC;PU, KY

出处：CHEMICAL SOCIETY REVIEWS 48 (1): 38-71 JAN 7 2019

摘要：Biophotonics as a highly interdisciplinary frontier often requires the assistance of optical agents to control the light pathways in cells, tissues and living organisms for specific biomedical applications. Organic semiconducting materials (OSMs) composed of pi-conjugated building blocks as the optically active components have recently emerged as a promising category of

biophotonic agents. OSMs possess common features including excellent optical properties, good photostability and biologically benign composition. This review summarizes the recent progress in the development of OSMs based on small-molecule fluorophores, aggregation-induced emission (AIE) dyes and semiconducting oligomer/polymer nanoparticles (SONs/SPNs) for advanced biophotonic applications. OSMs have been exploited as imaging agents to transduce biomolecular interactions into second near-infrared fluorescence, chemiluminescence, afterglow or photoacoustic signals, enabling deep-tissue ultrasensitive imaging of biological tissues, disease biomarkers and physiological indexes. By fine-tuning the molecular structures, OSMs can also convert light energy into cytotoxic free radicals or heat, allowing for effective cancer phototherapy. Due to their instant light response and efficient light-harvesting properties, precise regulation of biological activities using OSMs as remote transducers has been demonstrated for protein ion channels, gene transcription and protein activation. In addition to highlighting OSMs as a multifunctional platform for a wide range of biomedical applications, current challenges and perspectives of OSMs in biophotonics are discussed.

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17.被引频次：322

题目：CARBON CAPTURE AND CONVERSION USING METAL-ORGANIC FRAMEWORKS AND MOF-BASED MATERIALS

作者：DING, ML;FLAIG, RW;JIANG, HL;YAGHI, OM 出处：CHEMICAL SOCIETY REVIEWS 48 (10): 2783-2828 MAY 21 2019

摘要：Rapidly increasing atmospheric CO2 concentrations threaten human society, the natural environment, and the synergy between the two. In order to ameliorate the CO2 problem, carbon capture and conversion techniques have been proposed. Metal-organic framework (MOF)-based materials, a relatively new class of porous materials with unique structural features, high surface areas, chemical tunability and stability, have been extensively studied with respect to their applicability to such techniques. Recently, it has become apparent that the CO2 capture capabilities of MOF-based materials significantly boost their potential toward CO2 conversion. Furthermore, MOF-based materials' well-defined structures greatly facilitate the understanding of structure-property relationships and their roles in CO2 capture and conversion. In this review, we provide a comprehensive account of significant progress in the design and synthesis of MOF-based materials, including MOFs, MOF composites and MOF derivatives, and their application to carbon capture and conversion. Special emphases on the relationships between CO2 capture capacities of MOF-based materials and their catalytic CO2 conversion performances are discussed.

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18.被引频次：295
题目：PROGRESS AND PERSPECTIVES OF ELECTROCHEMICAL CO2 REDUCTION ON COPPER IN AQUEOUS ELECTROLYTE
作 者 ： NITOPI, S;BERTHEUSSEN, E;SCOTT, SB;LIU, XY;ENGSTFELD, AK;HORCH, S;SEGER, B;STEPHENS, IEL;CHAN, K;HAHN, C;NORSKOV, JK;JARAMILLO, TF;CHORKENDORFF, I
出处：CHEMICAL REVIEWS 119 (12): 7610-7672 JUN 26 2019
摘要：To date, copper is the only heterogeneous catalyst that has shown a propensity to produce valuable hydrocarbons and alcohols, such as ethylene and ethanol, from electrochemical CO2 reduction (CO2R). There are variety of factors that impact CO2R activity and selectivity, including the catalyst surface structure, morphology, composition, the choice of electrolyte ions and pH, and the electrochemical cell design. Many of these factors are often intertwined, which can complicate catalyst discovery and design efforts. Here we take a broad and historical view of these different aspects and their complex interplay in CO2R catalysis on Cu, with the purpose of providing new insights, critical evaluations, and guidance to the field with regard to research directions and best practices. First, we describe the various experimental probes and complementary theoretical methods that have been used to discern the mechanisms by which products are formed, and next we present our current understanding of the complex reaction networks for CO2R on Cu. We then analyze two key methods that have been used in attempts to alter the activity and selectivity of Cu: nanostructuring and the formation of bimetallic electrodes. Finally, we offer some perspectives on the future outlook for electrochemical CO2R.
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19.被引频次：292
题目：DUAL CROSSLINK HYDROGELS WITH METAL-LIGAND COORDINATION BONDS: TUNABLE DYNAMICS AND MECHANICS UNDER LARGE DEFORMATION
作者：ZHAO, JW;NARITA, T;CRETON, C
出处：SELF-HEALING AND SELF-RECOVERING HYDROGELS 285: 1-20 2020
摘要：Introducing additional physical and reversible crosslinks to a chemically crosslinked hydrogel is an interesting and viable alternative to increase the toughness of a hydrogel. Yet while in general the physical crosslink points provide dissipative mechanisms, there are still many details that are unknown in particular on the role that physical crosslinks play on the large strain behavior. We explore the mechanical properties in small and large strain of two dual crosslink gels

made from a random copolymer of poly(acrylamide-co-vinylimidazole) with a range of elastic moduli in the tens of kPa. The interaction between vinylimidazole groups and metal ions (Zn2+ and Ni2+) results in physical crosslink points and in a markedly stretch-rate-dependent mechanical behavior. While a main relaxation process is clearly visible in linear rheology and controls the small and intermediate strain properties, we find that the strain hardening behavior at stretches of lambda > 4 and the stretch at break lambda(b) are controlled by an additional longer-lived physical crosslinking mechanism that could be due to a clustering of physical crosslinks.

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20.被引频次：287

题目：CHEMODYNAMIC THERAPY: TUMOUR MICROENVIRONMENT-MEDIATED FENTON AND FENTON-LIKE REACTIONS

作者：TANG, ZM;LIU, YY;HE, MY;BU, WB

出处：ANGEWANDTE CHEMIE-INTERNATIONAL EDITION 58 (4): 946-956 JAN 21 2019

摘要：Tailored to the specific tumour microenvironment, which involves acidity and the overproduction of hydrogen peroxide, advanced nanotechnology has been introduced to generate the hydroxyl radical ((OH)-O-.) primarily for tumour chemodynamic therapy (CDT) through the Fenton and Fenton-like reactions. Numerous studies have investigated the enhancement of CDT efficiency, primarily the increase in the amount of (OH)-O-. generated. Notably, various strategies based on the Fenton reaction have been employed to enhance (OH)-O-. generation, including nanomaterials selection, modulation of the reaction environment, and external energy fields stimulation, which are discussed systematically in this Minireview. Furthermore, the potential challenges and the methods used to facilitate CDT effectiveness are also presented to support this cutting-edge research area. 地址： CHINESE ACAD SCI, STATE KEY LAB HIGH PERFORMANCE CERAM & SUPERFINE, SHANGHAI INST CERAM, SHANGHAI 200050, PEOPLES R CHINA;UNIV CHINESE ACAD SCI, BEIJING 100049, PEOPLES R CHINA;EAST CHINA NORMAL UNIV, SHANGHAI KEY LAB GREEN CHEM & CHEM PROC, SCH CHEM & MOL ENGN, SHANGHAI 200062, PEOPLES R CHINA
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21.被引频次：268

题目：DEFECT-RICH AND ULTRATHIN N DOPED CARBON NANOSHEETS AS ADVANCED TRIFUNCTIONAL METAL-FREE ELECTROCATALYSTS FOR THE ORR, OER AND HER

作者：JIANG, H;GU, JX;ZHENG, XS;LIU, M;QIU, XQ;WANG, LB;LI, WZ;CHEN, ZF;JI, XB;LI, J

出处：ENERGY & ENVIRONMENTAL SCIENCE 12 (1): 322-333 JAN 1 2019

摘要：Rational design and facile preparation of non-noble trifunctional electrocatalysts with high performance, low cost and strong durability for the oxygen reduction reaction (ORR), oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) are highly demanded, but

remain as a big challenge. Herein, we report a spontaneous gas-foaming method to prepare nitrogen doped ultrathin carbon nanosheets (NCNs) by simply pyrolysing a mixture of citric acid and NH4Cl. Under the optimized pyrolysis temperature (carbonized at 1000 degrees C) and mass ratio of precursors (1:1), the synthesized NCN-1000-5 sample possesses an ultrathin sheet structure, an ultrahigh specific surface area (1793 m(2) g(-1)), and rich edge defects, and exhibits low overpotential and robust stability for the ORR, OER and HER. By means of density functional theory (DFT) computations, we revealed that the intrinsic active sites for the ORR, OER and HER are the carbon atoms located at the armchair edge and adjacent to the graphitic N dopants. When practically used as a catalyst in rechargeable Zn-air batteries, a high energy density (806 W h kg(-1)), a low charge/discharge voltage gap (0.77 V) and an ultralong cycle life (over 330 h) were obtained at 10 mA cm(-2) for NCN-1000-5. This work not only presents a versatile strategy to develop advanced carbon materials with ultrahigh specific surface area and abundant edge defects, but also provides useful guidance for designing and developing multifunctional metal-free catalysts for various energy-related electrocatalytic reactions.

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22.被引频次：265

题目：UNDERSTANDING DEGRADATION MECHANISMS AND IMPROVING STABILITY OF PEROVSKITE PHOTOVOLTAICS

作者：BOYD, CC;CHEACHAROEN, R;LEIJTENS, T;MCGEHEE, MD

出处：CHEMICAL REVIEWS 119 (5): 3418-3451 SP. ISS. SI MAR 13 2019

摘要：This review article examines the current state of understanding in how metal halide perovskite solar cells can degrade when exposed to moisture, oxygen, heat, light, mechanical stress, and reverse bias. It also highlights strategies for improving stability, such as tuning the composition of the perovskite, introducing hydrophobic coatings, replacing metal electrodes with carbon or transparent conducting oxides, and packaging. The article concludes with recommendations on how accelerated testing should be performed to rapidly develop solar cells that are both extraordinarily efficient and stable.

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23.被引频次：258

题目：SOLAR ABSORBER MATERIAL AND SYSTEM DESIGNS FOR PHOTOTHERMAL WATER VAPORIZATION TOWARDS CLEAN WATER AND ENERGY PRODUCTION

作者：GAO, MM;ZHU, LL;PEH, CK;HO, GW

出处：ENERGY & ENVIRONMENTAL SCIENCE 12 (3): 841-864 MAR 1 2019

摘要：Photothermal materials with broad solar absorption and high conversion efficiency have recently attracted significant interest. They are becoming a fast-growing research focus in the area of solar-driven vaporization for clean water production. The parallel development of thermal management strategies through both material and system designs has further improved the overall efficiency of solar vaporization. Collectively, this green solar-driven water vaporization technology has regained attention as a sustainable solution for water scarcity. In this review, we will report the recent progress in solar absorber material design based on various photothermal conversion mechanisms, evaluate the prerequisites in terms of optical, thermal and wetting properties for efficient solar-driven water vaporization, classify the systems based on different photothermal evaporation configurations and discuss other correlated applications in the areas of desalination, water purification and energy generation. This article aims to provide a comprehensive review on the current development in efficient photothermal evaporation, and suggest directions to further enhance its overall efficiency through the judicious choice of materials and system designs, while synchronously capitalizing waste energy to realize concurrent clean water and energy production.

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24.被引频次：252

题目：METAL HALIDE PEROVSKITE NANOCRYSTALS: SYNTHESIS, POST-SYNTHESIS MODIFICATIONS, AND THEIR OPTICAL PROPERTIES

作者：SHAMSI, J;URBAN, AS;IMRAN, M;DE TRIZIO, L;MANNA, L

出处：CHEMICAL REVIEWS 119 (5): 3296-3348 SP. ISS. SI MAR 13 2019

摘要：Metal halide perovskites represent a flourishing area of research, which is driven by both their potential application in photovoltaics and optoelectronics and by the fundamental science behind their unique optoelectronic properties. The emergence of new colloidal methods for the synthesis of halide perovskite nanocrystals, as well as the interesting characteristics of this new type of material, has attracted the attention of many researchers. This review aims to provide an up-to-date survey of this fast-moving field and will mainly focus on the different colloidal synthesis approaches that have been developed. We will examine the chemistry and the capability of different colloidal synthetic routes with regard to controlling the shape, size, and optical properties of the resulting nanocrystals. We will also provide an up-to-date overview of their postsynthesis transformations, and summarize the various solution processes that are aimed at fabricating halide perovskite-based nanocomposites. Furthermore, we will review the fundamental optical properties of halide perovskite nanocrystals by focusing on their linear optical properties,

on the effects of quantum confinement, and on the current knowledge of their exciton binding energies. We will also discuss the emergence of nonlinear phenomena such as multiphoton absorption, biexcitons, and carrier multiplication. Finally, we will discuss open questions and possible future directions.

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25.被引频次：247

题目：A CRITICAL REVIEW OF THE ESTIMATION OF THE THERMODYNAMIC PARAMETERS ON ADSORPTION EQUILIBRIA. WRONG USE OF EQUILIBRIUM CONSTANT IN THE VANT HOOF EQUATION FOR CALCULATION OF THERMODYNAMIC PARAMETERS OF ADSORPTION

作者：LIMA, EC;HOSSEINI-BANDEGHARAEI, A;MORENO-PIRAJAN, JC;ANASTOPOULOS, I JOURNAL OF MOLECULAR LIQUIDS 273: 425-434 JAN 2019

摘要：In the adsorption literature, the Van't Hoff equation is used in different manners without any criteria about the concepts of physical-chemistry of equilibrium for calculation of thermodynamic parameters of adsorption. Indeed, the equilibrium constant (K) should be dimensionless for being used in the Van't Hoff equation. However, this is not a simple adjustment of units, as being spread in the literature, to become K dimensionless. In this paper, it will be calculated the equilibrium constants using numeric examples and show the flaws of the thermodynamics calculations, when the value of K is wrongly calculated, and what are the expected results of the changes in enthalpy (Delta H degrees) and changes in the entropy (Delta S degrees) that are spread in the literature. (C) 2018 Published by Elsevier B.V.

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ESI HIGHLY CITED PAPERS

(Chemistry)

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

1.被引频次：17119
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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2.被引频次：16082
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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3.被引频次：8654
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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4.被引频次：7432
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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5.被引频次：7245
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：6691
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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7.被引频次：6607

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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8.被引频次：6585

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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9.被引频次：6376

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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10.被引频次：6354

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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ENGLAND;TOIN UNIV YOKOHAMA, GRAD SCH ENGN, AOBA KU, YOKOHAMA, KANAGAWA 2258503, JAPAN;NATL INST ADV IND SCI & TECHNOL, RES CTR PHOTOVOLTA TECHNOL, TSUKUBA, IBARAKI 3058565, JAPAN
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11.被引频次：6325
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
地址：UPPSALA UNIV, DEPT PHYS & ANALYT CHEM, SE-75105 UPPSALA, SWEDEN;KTH ROYAL INST TECHNOL, DEPT CHEM, SE-10044 STOCKHOLM, SWEDEN;DALIAN UNIV TECHNOL, STATE KEY LAB FINE CHEM, DUT KTH JOINT EDUC & RES CTR MOL DEVICES, DALIAN 116012, PEOPLES R CHINA;SWEREA IVF AB, SE-43122 MOLNDAL, SWEDEN
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12.被引频次：6141
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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13.被引频次：5974
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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电子邮件地址：nslewis@caltech.edu

14.被引频次：5565
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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15.被引频次：5227
题目：THE ORCA PROGRAM SYSTEM
作者：NEESE, F
出处：WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE 2 (1): 73-78 JAN-FEB 2012
摘要：ORCA is a general-purpose quantum chemistry program package that features virtually all modern electronic structure methods (density functional theory, many-body perturbation and coupled cluster theories, and multireference and semiempirical methods). It is designed with the aim of generality, extendibility, efficiency, and user friendliness. Its main field of application is larger molecules, transition metal complexes, and their spectroscopic properties. ORCA uses standard Gaussian basis functions and is fully parallelized. The article provides an overview of its current possibilities and documents its efficiency. (c) 2011 John Wiley & Sons, Ltd.
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电子邮件地址：neese@thch.uni-bonn.de

16.被引频次：5163
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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17.被引频次：4962
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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18.被引频次：4749
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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19.被引频次：4602

题目：METAL-ORGANIC FRAMEWORK MATERIALS AS CHEMICAL SENSORS

作者：KRENO, LE;LEONG, K;FARHA, OK;ALLENDORF, M;VAN DUYNE, RP;HUPP, JT

出处：CHEMICAL REVIEWS 112 (2): 1105-1125 SP. ISS. SI FEB 2012

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20.被引频次：4572

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

地址：UNIV MICHIGAN, DEPT CHEM, ANN ARBOR, MI 48109 USA

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21.被引频次：4404

题目：METAL-ORGANIC FRAMEWORKS FOR SEPARATIONS

作者：LI, JR;SCULLEY, J;ZHOU, HC

出处：CHEMICAL REVIEWS 112 (2): 869-932 SP. ISS. SI FEB 2012

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22.被引频次：4379

题目：PHYSISORPTION OF GASES, WITH SPECIAL REFERENCE TO THE EVALUATION OF SURFACE AREA AND PORE SIZE DISTRIBUTION (IUPAC TECHNICAL REPORT)

作者：THOMMES, M;KANEKO, K;NEIMARK, AV;OLIVIER, JP;RODRIGUEZ-REINOSO, F;ROUQUEROL, J;SING, KSW

出处：PURE AND APPLIED CHEMISTRY 87 (9-10): 1051-1069 OCT 2015

摘要：Gas adsorption is an important tool for the characterisation of porous solids and fine powders. Major advances in recent years have made it necessary to update the 1985 IUPAC manual on Reporting Physisorption Data for Gas/Solid Systems. The aims of the present document are to clarify and standardise the presentation, nomenclature and methodology associated with the application of physisorption for surface area assessment and pore size analysis and to draw attention to remaining problems in the interpretation of physisorption data.

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23.被引频次：4374

题目：INTERFACE ENGINEERING OF HIGHLY EFFICIENT PEROVSKITE SOLAR CELLS

作者：ZHOU, HP;CHEN, Q;LI, G;LUO, S;SONG, TB;DUAN, HS;HONG, ZR;YOU, JB;LIU, YS;YANG, Y

出处：SCIENCE 345 (6196): 542-546 AUG 1 2014

摘要：Advancing perovskite solar cell technologies toward their theoretical power conversion efficiency (PCE) requires delicate control over the carrier dynamics throughout the entire device. By controlling the formation of the perovskite layer and careful choices of other materials, we suppressed carrier recombination in the absorber, facilitated carrier injection into the carrier transport layers, and maintained good carrier extraction at the electrodes. When measured via reverse bias scan, cell PCE is typically boosted to 16.6% on average, with the highest efficiency of similar to 19.3% in a planar geometry without antireflective coating. The fabrication of our perovskite solar cells was conducted in air and from solution at low temperatures, which should simplify manufacturing of large-area perovskite devices that are inexpensive and perform at high levels.

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24.被引频次：4332
题目：HONEYCOMB CARBON: A REVIEW OF GRAPHENE
作者：ALLEN, MJ;TUNG, VC;KANER, RB
出处：CHEMICAL REVIEWS 110 (1): 132-145 JAN 2010
地址：UNIV CALIF LOS ANGELES, DEPT CHEM & BIOCHEM, LOS ANGELES, CA 90095 USA;UNIV CALIF LOS ANGELES, CALIF NANOSYST INST, LOS ANGELES, CA 90095 USA;UNIV CALIF LOS ANGELES, DEPT MAT SCI & ENGN, LOS ANGELES, CA 90095 USA

25.被引频次：4304
题目：CARBON DIOXIDE CAPTURE IN METAL-ORGANIC FRAMEWORKS
作者：SUMIDA, K;ROGOW, DL;MASON, JA;MCDONALD, TM;BLOCH, ED;HERM, ZR;BAE, TH;LONG, JR
出处：CHEMICAL REVIEWS 112 (2): 724-781 SP. ISS. SI FEB 2012
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AIAA、IAF 最新会议

AIAA

（AIAA 来源：http://www.aiaa.org/）

1.会议名称：2021 Aerospace Spotlight Awards Gala
会议时间： 18 August 2021,
会议地点：Washington, D.C.
会议简介：On 18 August 2021, AIAA will host an extraordinary evening to inspire and advance the future of aerospace. From the important missions that reinvent our national uses of air and space, to the innovative new applications that enhance everyday living, AIAA recognizes individuals and institutions that are making the world safer, more connected, and more prosperous.
链接：
https://www.aiaa.org/events-learning/event/2021/08/18/default-calendar/2021-aerospace-spotlight-awards-gala

2.会议名称：3rd International Academy of Astronautics (IAA) Conference on Space Situational Awareness
会议时间：13 September - 15 September 2021
会议地点：GMV, Madrid, Spain
会议简介：The foremost purpose of Space Situational Awareness (SSA) is to provide decision-making processes with a quantifiable and timely body of evidence (predictive/imminent/forensic) of behavior(s) attributable to specific space domain threats and hazards. The conference will cover broad-ranging technical and policy related aspects associated with the topic of SSA. Over the past two decades, SSA has evolved into a high-impact, multidisciplinary field of research. The magnitude and complexity of its constituent lines of inquiry are growing at rapid pace, driven by the increasing number of objects of interest, including resident space objects: RSOs (a collective term for active spacecraft and space debris) as well as near Earth objects: NEOs (comets and asteroids in Earth’s vicinity). Combining its various “notions”, SSA today spans research in areas of RSO/NEO sensing, identification, forecasting, tracking, association, risk assessment, resource allocation, spacecraft control, information & communication, proximity operations, debris removal, space weather, drag-controlled re-entry, alternative (non-propulsive) deorbiting technologies, liability and insurance issues and a host of other related topics. Continued sustainable access and utilization of space relies on the awareness of its environment, both from the perspective of human operators on the ground and autonomous spacecraft during flight. Moreover, as the nature and number of participants utilizing the space environment grows, there is critical need for steadfast governance driven by a coherent space policy.
链接：
https://www.aiaa.org/events-learning/event/2021/09/13/default-calendar/3rd-international-academ

y-of-astronautics-(iaa)-conference-on-space-situational-awareness

3.会议名称：2021 AIAA Defense and Security Forum (AIAA DEFENSE Forum)
会议时间：20 September - 22 September 2021
会议地点：Laurel, Maryland, USA
会议简介：The 2021 forum will bring together government, military, industry, and academia to discuss the strategic, programmatic, and technical topics and policy issues in aerospace and defense.
链接：
https://www.aiaa.org/events-learning/event/2021/09/20/default-calendar/2021-aiaa-defense-and-security-forum-(aiaa-defense-forum)

4.会议名称：AIAA International Space Planes and Hypersonic Systems and Technologies Conference
会议时间：15 November - 17 November 2021
会议地点：Las Vegas, Nevada & ONLINE
会议简介：The 24th AIAA International Space Planes and Hypersonic Systems and Technologies Conference, as a part of ASCEND 2021, provides a forum for discussion and exchange of information for attendees from across the globe about leading-edge research and development activities associated with space planes and hypersonic atmospheric flight vehicles and the technologies underpinning these capabilities. Presentations will be provided on national programs from North America, South America, Australia, Europe, and Asia and multiple opportunities for international collaboration will be discussed.
链接：
https://www.aiaa.org/events-learning/event/2021/11/15/default-calendar/24th-aiaa-international-space-planes-and-hypersonic-systems-and-technologies-conference

IAF

（IAF 来源：http://www.iafastro.org/）

会议名称：THE GLOBAL SPACE EXPLORATION CONFERENCE 2021
会议时间： 14－18 June 2021
会议地点：St. Petersburg, Russian Federation
会议简介：The Conference, co-organized by the International Astronautical Federation (IAF) and ROSCOSMOS, will bring together leaders and decision-makers within the science and human exploration community － engineers, scientists, entrepreneurs, educators, agency representatives and policy makers. The leaders in the field will converge in St. Petersburg to discuss recent results, current challenges and innovative solutions and it will contain several opportunities to learn about how space exploration investments provide benefits as well as discuss how those benefits can be increased through thoughtful planning and cooperation.
链接：https://www.iafastro.org/events/global-series-conferences/glex-2021/

ACM 最新会议

来源：http://www.acm.org/

1.会议名称：2021 4th International Conference on Robotics and Mechantronics
会议时间：May 28-30th, 2021
会议地点： Paris, France
会议简介：Nowadays, Automation and Mechatronics Engineering play an increasingly important role in both control and engineering applications. In the real world, the environment is complex and dynamics. As such, the automation systems should learn and adapt accordingly and more efforts should be focused on the methodology of the learning system on one hand. For example, fast adaptation and self-organizing capability are highly desired and research activities on this type of development should be expedited. On the other hand, one should leverage on artificial intelligence and machine learning to enhance their performance. Towards this end, the 2021 4th International Conference on Robotics and Mechantronics (ICRoM 2021) will be organized.
ICRoM 2021 will be held during May 28-30th, 2021 in Paris, France. The main goal of ICRoM 2021 is to address latest original results in advanced intelligent control of automation systems, including both theoretical advances and practical implementations, which are becoming more and more popular in industry and in our daily lives. The ICRoM 2021will provide a premier interdisciplinary platform for scientists, researchers, industry leaders, engineers and educators throughout the world to present and discuss the most recent innovations, trends, concerns, as well as practical challenges encountered, and streamline solutions in the fields of Robotics and Mechantronics. The meeting will provide an opportunity to highlight recent developments and to identify emerging and future areas of growth in Robotics and Mechantronics.
链接：http://www.icrom.org/

2.会议名称：2021 The 3rd International Conference on Composite Materials Science and Technology (ICCMST 2021)
会议时间：June 17-21, 2021.
会议地点： Cavtat, Croatia
会议简介：2021 The 3rd International Conference on Composite Materials Science and Technology (ICCMST 2021) will be held in Cavtat, Croatia, during June 17-21, 2021. It is a great pleasure for ICCMST to invite prospective authors initiating the discussion on the challenges that need to be timely overcome and addressing key questions in the field of Composite Materials Science and Technology.
ICCMST is a remarkable event which facilitates the exchanges of ideas, novel and practical techniques and applications in various fields of advanced materials including but limited to composite materials and nanomaterials, chemical and materials engineering, nanotechnology etc.
链接：http://iccmst.org/

3.会议名称： 2021 4th International Conference on Mathematics and Statistics (ICoMS 2021)
会议时间：June 24-26, 2021.
会议地点： Paris, France
会议简介：ICoMS 2021 is organized to bring together worldwide leading researchers and practitioners interested in advancing the state of the art in Mathematics and Statistics, for exchanging knowledge that encompasses a broad range of disciplines among various distinct communities. It is hoped that researchers and practitioners will bring new prospects for collaboration across disciplines and gain inspiration to facilitate novel breakthroughs. The themes for this conference are thus focused on "Statisticsof Stochastic Processes and Algorithms".
The annually held conference is expected to provide an opportunity for the researchers to meet and discuss the latest solutions, scientific results and methods in solving intriguing problems in the fields of Mathematics and Statistics. The conference programme will include prominent keynote speakers, invited speakers and regular paper presentations in parallel tracks. The General Chairs, along with the entire team cordially invite you to submit your latest research results and to take part in the upcoming conference, to be held during June 24-26, 2021 in Paris, France.
链接：http://www.icoms.org/

4.会议名称：The 13th International Conference on Computer Modeling and Simulation (ICCMS 2021)
会议时间： June 25-27, 2021.
会议地点： Australia, University of Wollongong
会议简介：ICCMS is annual event with a rich history of providing quality services for the international research, academic and industry communities in Computer Modeling and Simulation over a decade, particularly in the Asian-Pacific region.
The three-day event features keynote speeches and invited talks on Computer Modeling and Simulation, regular paper presentations, as well as tutorials delivered by leading experts in the respective fields. Additionally, a city tour in Melbourne, Australia will be organized during the conference.
During the conference you will not only have the opportunity to experience the link between theory and practice but you will also be part of an international network of researchers and lecturers in the field of Computer Modeling and Simulation.
链接：http://www.iccms.org/index.html

5.会议名称：2021 5th High Performance Computing and Cluster Technologies Conference
会议时间：July 02-04, 2021
会议地点：Ocean University of China, Qingdao, China
会议简介：The aim as well as objective of HPCCT 2021 is to present the latest research and results of scientists related to High Performance Computing and Cluster Technologies topics. This conference provides opportunities for the delegates to exchange new ideas face-to-face, to establish business or research relations as well as to find global partners for future collaborations. We hope that the conference results will lead to significant contributions to **the knowledge in** these up-to-date scientific fields.
链接：http://hpcct.org/

6.会议名称：The 2021 8th International Conference on Management of e-Commerce and e-Government (ICMECG 2021)
会议时间：July 04-06, 2021
会议地点：Jeju Island, South Korea
会议简介：As an easier and more efficient way to handle business and affairs, e-Commerce and e-Government have been applied extensively all over the world and became an indispensable part of daily life. Organized by International Economics Development and Research Center, The 2021 8th International Conference on Management of e-Commerce and e-Government (ICMECG 2021) will be held in Jeju Island, South Korea during July 04-06, 2021. It aims to provide a high quality platform for researchers, practitioners and policy makers from all over the world to present their latest research findings, ideas, and applications in the related fields of e-Commerce and e-Government. Featured with keynote session, technical session and social networking event, ICMECG 2021 will afford the delegates an unparalleled opportunity to communicate with qualified professionals and build future partnership.
链接：http://www.icmecg.net/

7.会议名称：2021 7th International Conference on Computer Technology Applications (ICCTA 2021, former ICCIT)
会议时间：July 13-15, 2021
会议地点：Vienna, Austria
会议简介：ICCTA is the premier for the presentation and exchange of past experiences and new advances and research results in the field of theoretical and industrial experience. The conference welcomes contributions which promote the exchange of ideas and rational discourse between educators and researchers all over the world.
链接：http://www.iccit.org/index.html

8.会议名称：2021 5th International Conference on Education and Multimedia Technology (ICEMT 2021)
会议时间：July 23-25, 2021
会议地点： Kyoto, Japan
会议简介：ICEMT 2021 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 Education and Multimedia Technology, 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 Education, Multimedia Technology and related areas.
链接：http://www.icemt.org/index.html

9.会议名称： 2021 International Symposium on Biomedical Engineering and Computational Biology (BECB 2021)
会议时间： August 13-15, 2021
会议地点：Online
会议简介：The BECB is a flagship annual international conference on biomedical engineering and bioinformatics, promoting all aspects of theory, algorithm design, applications and related

emerging techniques. As a tradition, the BECB 2021 will co-locate a large number of topics within or related to biomedical engineering and bioinformatics, thereby providing a unique platform for promoting cross-fertilization and collaboration. The BECB 2021 will be featured by keynote speeches, oral presentations and poster sessions.

链接：https://www.becbinfo.com/#/

10.会议名称：2021 4th International Conference on Information Management and Management Science (IMMS 2021)

会议时间：the 27th to the 29th of August, 2021.

会议地点：Chengdu, China

会议简介：Over the past years, interests on relevant topics has remarkably increased. Novel ideas and impressive effort on data analysis and software engineering, intelligent business and enterprise management, product design and management, and modern information technology and applications are the evidence of good attempts and significant progress in the fields. The main aim of IMMS 2021 has always been bringing together a large group of researchers, scientists, academics, engineers, directors, managers, consultants and analysts in the area of information management and management science from all over the world, to share much more than research findings, among other things, culture and history. It provides a high-standard international forum for exchanging brilliant ideas and experience. The distinguished speakers have provided different perspectives of research and results in different countries. All the full papers will go through a rigorous blind peer-reviewing process.

链接：http://www.imms.net/

IQPC 最新国防会议(Defence)

IQPC 来源：http://www.iqpc.com/

1.会议名称：Future Amphibious Force 2021
会议时间：18-19 May
会议地点：online
会议简介：Hosted with the support of the Royal Marines, Future Amphibious Force 2021 will take place at an exciting time for UK amphibious capability, as the Royal Marines forge ahead with a major transformation programme to develop the Future Commando Force.
From 18-19 May, Future Amphibious Force 2021 will bring together international leaders to contribute and share knowledge on the future nature and utility of amphibiosity, as well as how their services are preparing for change. The two-day online conference will foster an environment of collaboration, providing an opportunity for participation in interactive discussions and high-level debates.
Our speakers will share their assessments of the changing threats faced by navies and amphibious forces (including A2/AD); priority capability areas for development, and how Marine forces are adapting to this new world through the use of new disruptive technologies.
链接：
https://www.defenceiq.com/events-future-amphibious-force-online/?utm_medium=portal&mac=IQPCCORP

2.会议名称：Defence iQ's Military Flight Training conference
会议时间：29 June - 01 July, 2021
会议地点：online
会议简介：Defence iQ's Military Flight Training conference will be taking place from 29 June - 01 July online.
Concurrent with today’s operational context, Military Flight Training 2021 will discuss key challenge areas including: training for contested and degraded environments, delivering LVC in mixed inventories of new and legacy platforms, solving red air deficiency, LVC interoperability, rotary-wing training, recruitment & retention, operational conversion training and crew resource management, integrated synthetic/virtual training capabilities, and effective threat emulations.
链接：
https://www.defenceiq.com/events-militaryflighttraining/?utm_medium=portal&mac=IQPCCORP

3.会议名称：Space Operations Summit
会议时间：07 - 08 September, 2021
会议地点：London
会议简介：Since Defence IQ launched the inaugural Space Operations Summit in 2019, NATO

has approved its first space policy and recognised space as an operational domain. These developments emphasise that the outcome of future multi-domain operations will depend on NATO's ability both to generate capability in space and to leverage space-based capabilities across the joint environment.

Space Operations 2020 offers a platform for military space professionals, joint-space users, aerospace leaders and space SMEs to translate space concepts into robust capabilities. The conference is also committed to enhancing dialogue on the space industrial base and to enabling the agile acquisition processes that can rapidly and iteratively build capability in NATO's newest warfighting domain.

The workshop and opening plenary sessions acknowledge that our ability to operate in and from space depends on improved access to space. For the military user, that means leveraging partnerships with commercial launch service providers to generate a reliable, affordable and repeatable launch capability. Only through improved access to launch can defence effectively build capability in space, enhancing SSA, improving resiliency for space-based systems and fielding small-sat development.

Last, but just as important, the programme will look at the delivery of effect from space. As multi-domain thinking continues to mature, it is vital that we consider how to integrate space capabilities and effects with forces operating in the air, on land, at sea and in cyberspace.

链接：

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

4.会议名称：Big Data for Defence

会议时间：27 - 28 September, 2021

会议地点：London, United Kingdom

会议简介：As the variety, volume, veracity, and velocity of data is undergoing a rapid transformation and aggravating the cognitive burden on the Warfighter, armed forces require technologies to store, process, verify, and disseminate actionable intelligence at pace. It is widely accepted that decision-making in the future information-dominated battlespace will depend on big data analytics, AI/ML, and data connectivity.

However, existing institutions and mechanisms are largely rooted in outdated conventions, which impede rapid exploitation and integration of disruptive technologies. In order to retain the competitive edge against increasingly capable opponents, defence leaders must embrace technology offered by the civil sector and deliver decisive capability into the hands of the Warfighter.

Over the course of 3 days, the conference will explore ways to gain and retain the information advantage through disruptive innovation and big data analytics – addressing cloud computing, the acquisition of data from disparate sources, data validation, visualisation, accelerated and autonomous decision-making, and network resilience through cyber defence mechanisms. The conference programme will feature case studies, demonstrating adoption and applications of advanced military software.

链接：

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

5.会议名称：Offshore Patrol Vessels International

会议时间：27 - 30 September, 2021

会议地点：Online Event

会议简介：Now well established as the leading conference for Navies, Coast Guards, related maritime organisations and Industry to discuss these versatile platforms, OPV International will evaluate multi-role vessels through the lens of their whole life cycle. In doing so it can be a powerful vehicle for meaningful consensus between experts from across the community to share challenges and contribute to finding the most effective solutions.

This year across three days of presentations, panel discussions and immersive networking opportunities, OPV International will discuss current and ongoing procurement programs as well as operational challenges, lessons learned and future technologies. Casting its attention towards the advent of the Digital Age for the first time, it will provide an opportunity for experts from across the various stages of the OPV life cycle and supply chain to impact the development of what is the fastest-growing sector of the Naval market.

Join us in September 2021 as we work to maximise situational awareness, upgrade inherent baseline capability and deliver a continuous patrol function for the OPV.

链接：

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

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