图书情报专题研究

最新学科研究热点与前沿

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前　言

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

本期收集整理了如下七个方面的热点文献和前沿信息：

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

2、IEL Top25，IEL 数据库下载最多的 25 篇论文；

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

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

5、AIAA、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

2022 年 3 月

目 录

NatureLatest Research(Chemistry)

来源：https://www.nature.com/physics/

1. 标题：Kinetic resolution of cyclic benzylic azides enabled by site- and enantioselective C(sp3)–H oxidation
作者：Pengbo Ye, Aili Feng, Lin Wang, Min Cao, Rongxiu Zhu & Lei Liu
摘要：Catalytic nonenzymatic kinetic resolution (KR) of racemates remains one of the most powerful tools to prepare enantiopure compounds, which dominantly relies on the manipulation of reactive functional groups. Moreover, catalytic KR of organic azides represents a formidable challenge due to the small size and instability of the azido group. Here, an effective KR of cyclic benzylic azides through site- and enantioselective C(sp3)–H oxidation is described. The manganese catalyzed oxidative KR reaction exhibits good functional group tolerance, and is applicable to a range of tetrahydroquinoline- and indoline-based organic azides with excellent site- and enantio-discrimination. Computational studies elucidate that the effective chiral recognition is derived from hydrogen bonding interaction between substrate and catalyst.
链接：https://www.nature.com/articles/s41467-022-29319-z

2. 标题：Pomegranate fruit juice adulteration with apple juice: detection by UV–visible spectroscopy combined with multivariate statistical analysis
作者：Lucia Pappalardo
摘要：Pomegranate is rich in high value nutritional substances known to be beneficial against several diseases and its use in medicine is known since ancient times. Due to its properties and delicious taste, pomegranate fresh fruit juices demand has been growing worldwide and its adulteration is becoming a problem. Low-cost, user friendly and fast detection methods are therefore desirable in order to easily and rapidly detect adulteration of short shelf-life fresh fruit juices. For this purpose fresh squeezed arils pomegranate juice samples adulterated with less expensive apple juice concentrate were investigated by UV–visible spectroscopy combined with multivariate statistical analysis. Unsupervised principle component analysis (PCA), supervised projection to latent structure discriminant analysis (PLS-DA) and orthogonal projection to latent structure discriminant analysis (OPLS-DA) were performed on the full spectra. OPLS-DA analysis of UV–visible spectra proved to be a suitable method to detect pomegranate juices adulterated by more than 20% v/v apple juice concentrate.
链接：https://www.nature.com/articles/s41598-022-07979-7

3. 标题：Sticky-MARTINI as a reactive coarse-grained model for molecular dynamics simulations of silica polymerization
作者：André P. Carvalho, Sérgio M. Santos, Germán Pérez-Sánchez, José D. Gouveia, José R. B. Gomes & Miguel Jorge
摘要：We report a molecular modeling paradigm to describe silica polymerization reactions in

aqueous solutions at conditions that are representative of realistic experimental processes like biosilicification or porous silica synthesis – i.e. at close to ambient temperatures and over a wide range of pH. The key point is to describe the Si-O-Si chemical bond formation and breakage processes through a continuous potential with a balance between attractive and repulsive interactions between suitably placed virtual sites and sticky particles. The simplicity of the model, its applicability in standard parallelized molecular dynamics codes, and its compatibility with the widely used MARTINI coarse-grained force-field allows for the study of systems containing millions of atoms over microsecond time scales. The model is calibrated to match experimental results for the temporal evolution of silica polymerization in aqueous solution close to the isoelectric point, and can describe silica polymerization and self-assembly processes during encapsulation of a surfactant micelle.

链接：https://www.nature.com/articles/s41524-022-00722-w

4. **标题：**Structural and dynamic properties of eutectic mixtures based on menthol and fatty acids derived from coconut oil: a MD simulation study

作 者： Samaneh Barani pour, Jaber Jahanbin Sardroodi, Alireza Rastkar Ebrahimzadeh & Mohammad Sadegh Avestan

摘要：The structural and dynamical properties of the binary mixture of Menthol (MEN) and Fatty acids (FAs) were investigated using molecular dynamics simulations. To this end, the relationship between the structural and dynamical properties of the eutectic mixtures of MEN and FAs with different molar percentages of FAs are studied. Structural properties of the eutectic mixtures were characterized by calculating the combined distribution functions (CDFs), radial distribution functions (RDFs), angular distribution functions (ADFs), hydrogen bonding networks, and spatial distribution functions (SDF). Additionally, our Results indicated robust interactions between menthol and Caprylic acid molecules Finally, the transport properties of the mixtures were investigated using the mean square displacement (MSD) of the centers of mass of the species, self-diffusion coefficients and vector reorientation dynamics (VRD) of bonds. Overall, our simulation results indicated that intermolecular interactions have a significant effect on the dynamic properties of species.

链接：https://www.nature.com/articles/s41598-022-09044-9

5. **标题：**Topoarchitected polymer networks expand the space of material properties

作者：Xiao Liu, Jingping Wu, Keke Qiao, Guohan Liu, Zhengjin Wang, Tongqing Lu, Zhigang Suo & Jian Hu

摘要：Many living tissues achieve functions through architected constituents with strong adhesion. An Achilles tendon, for example, transmits force, elastically and repeatedly, from a muscle to a bone through staggered alignment of stiff collagen fibrils in a soft proteoglycan matrix. The collagen fibrils align orderly and adhere to the proteoglycan strongly. However, synthesizing architected materials with strong adhesion has been challenging. Here we fabricate architected polymer networks by sequential polymerization and photolithography, and attain adherent interface by topological entanglement. We fabricate tendon-inspired hydrogels by embedding hard blocks in topological entanglement with a soft matrix. The staggered architecture and strong adhesion enable high elastic limit strain and high toughness simultaneously. This combination of

attributes is commonly desired in applications, but rarely achieved in synthetic materials. We further demonstrate architected polymer networks of various geometric patterns and material combinations to show the potential for expanding the space of material properties.

链接：https://www.nature.com/articles/s41467-022-29245-0

6. **标 题 ：** Combining elemental and immunochemical analyses to characterize diagenetic alteration patterns in ancient skeletal remains

作者：L. Gatti, Federico Lugli, Giorgia Sciutto, M. Zangheri, S. Prati, M. Mirasoli, S. Silvestrini, S. Benazzi, T. Tütken, K. Douka, C. Collina, F. Boschin, M. Romandini, P. Iacumin, M. Guardigli, A. Roda & R. Mazzeo

摘要：Bones and teeth are biological archives, but their structure and composition are subjected to alteration overtime due to biological and chemical degradation postmortem, influenced by burial environment and conditions. Nevertheless, organic fraction preservation is mandatory for several archeometric analyses and applications. The mutual protection between biomineral and organic fractions in bones and teeth may lead to a limited diagenetic alteration, promoting a better conservation of the organic fraction. However, the correlation between elemental variations and the presence of organic materials (e.g., collagen) in the same specimen is still unclear. To fill this gap, chemiluminescent (CL) immunochemical imaging analysis has been applied for the first time for collagen localization. Then, Laser Ablation–Inductively Coupled Plasma–Mass Spectrometry (LA–ICP–MS) and CL imaging were combined to investigate the correlation between elemental (i.e., REE, U, Sr, Ba) and collagen distribution. Teeth and bones from various archeological contexts, chronological periods, and characterized by different collagen content were analyzed. Immunochemical analysis revealed a heterogeneous distribution of collagen, especially in highly degraded samples. Subsequently, LA–ICP–MS showed a correlation between the presence of uranium and rare earth elements and areas with low amount of collagen. The innovative integration between the two methods permitted to clarify the mutual relation between elemental variation and collagen preservation overtime, thus contributing to unravel the effects of diagenetic alteration in bones and teeth.

链接：https://www.nature.com/articles/s41598-022-08979-3

7. **标 题 ：** Cobalt(II)–tetraphenylporphyrin-catalysed carbene transfer from acceptor–acceptor iodonium ylides via N-enolate–carbene radicals

作者：Roel F. J. Epping, Mees M. Hoeksma, Eduard O. Bobylev, Simon Mathew & Bas de Bruin

摘要：Square-planar cobalt(II) systems have emerged as powerful carbene transfer catalysts for the synthesis of numerous (hetero)cyclic compounds via cobalt(III)–carbene radical intermediates. Spectroscopic detection and characterization of reactive carbene radical intermediates is limited to a few scattered experiments, centered around monosubstituted carbenes. Here, we reveal the formation of disubstituted cobalt(III)–carbene radicals derived from a cobalt(II)–tetraphenylporphyrin complex and acceptor–acceptor λ 3-iodaneylidenes (iodonium ylides) as carbene precursors and their catalytic application. Iodonium ylides generate biscarbenoid species via reversible ligand modification of the paramagnetic cobalt(II)–tetraphenylporphyrin complex catalyst. Two interconnected catalytic cycles are involved in the overall mechanism, with a monocarbene radical and an N-enolate–carbene radical

intermediate at the heart of each respective cycle. Notably, N-enolate formation is not a deactivation pathway but a reversible process, enabling transfer of two carbene moieties from a single N-enolate–carbene radical intermediate. The findings are supported by extensive experimental and computational studies.

链接：https://www.nature.com/articles/s41557-022-00905-4

8. **标题：**Preparation of amine- and ammonium-containing polysilsesquioxane membranes for CO2 separation

作 者： Joji Ohshita, Takatoshi Okonogi, Kohei Kajimura, Katsuhiro Horata, Yohei Adachi, Masakoto Kanezashi & Toshinori Tsuru

摘要：Amine-containing polysilsesquioxane (PSQ) membranes were studied with regard to their CO2 separation ability. PSQ membranes were prepared by the sol–gel process using three amine-containing monomers, bis(triethoxysilylpropyl)amine (BTESPA), (aminopropyl)triethoxysilane (APTES), and (aminoethylaminopropyl)triethoxysilane (AEAPTES), to examine the relationship between precursor structure and membrane performance. The CO2 permeances of the membranes prepared by 1:1 copolymerization with bis(triethoxysilyl)ethane increased in the order of AEAPTES-derived membranes < APTES-derived membranes < BTESPA-derived membranes, and their CO2/N2 permselectivities decreased in the same order. On the basis of density functional theory calculations on model systems and nitrogen adsorption-desorption experiments of the PSQ gels, it was found that CO2 affinity and porosity of the membranes were important factors affecting CO2 separation performance. Copolymerization under acidic conditions resulted in the formation of ammonium-containing membranes with improved CO2 permeances and acceptable CO2/N2 permselectivities.

链接：https://www.nature.com/articles/s41428-022-00635-x

9. **标题：**Complementary catalysis and analysis within solid state additively manufactured metal micro flow reactors

作者：T. Monaghan, M. J. Harding, S. D. R. Christie, R. A. Harris & R. J. Friel

摘要：Additive Manufacturing is transforming how researchers and industrialists look to design and manufacture chemical devices to meet their specific needs. In this work, we report the first example of a flow reactor formed via the solid-state metal sheet lamination technique, Ultrasonic Additive Manufacturing (UAM), with directly integrated catalytic sections and sensing elements. The UAM technology not only overcomes many of the current limitations associated with the additive manufacturing of chemical reactionware but it also significantly increases the functionality of such devices. A range of biologically important 1, 4-disubstituted 1, 2, 3-triazole compounds were successfully synthesised and optimised in-flow through a Cu mediated Huisgen 1, 3-dipolar cycloaddition using the UAM chemical device. By exploiting the unique properties of UAM and continuous flow processing, the device was able to catalyse the proceeding reactions whilst also providing real-time feedback for reaction monitoring and optimisation.

链接：https://www.nature.com/articles/s41598-022-09044-9

10. 标题：Hydrogen generation from biomass by pyrolysis

作者：Gartzen Lopez, Laura Santamaria, Angeliki Lemonidou, Shuming Zhang, Chunfei Wu, Ayesha T. Sipra & Ningbo Gao

摘要：The growing environmental concerns associated with global warming along with the exponential rise in energy demand are boosting the production of clean energy. The combined process of biomass pyrolysis and in-line catalytic steam reforming is a promising alternative for the selective production of hydrogen from renewable sources. This Primer provides a general overview of the fundamental aspects that influence the hydrogen production potential of the process. Recent research studies and their main findings are highlighted. The current challenges and limitations of the process and ways to optimize the biomass-derived products of steam reforming are discussed. Finally, we evaluate progress toward the industrial scalability of the process.

链接：https://www.nature.com/articles/s43586-022-00097-8

11. 标题：In-operando analysis of the corrosion patterns and rates under magnetic fields using metallic film

作者：Cirlei Igreja Nascimento Mitre, Giancarlo Tosin & Luiz Alberto Colnago

摘要：Magnets, or electromagnets, are common components in everyday appliances and are widely used in medicine, industries, transportation, and electrical power systems. It is known that the magnetic field (B) can mitigate or aggravate metallic corrosion; however, this apparent contradictory effect is still not fully understood. In this study, we demonstrate a simple method to monitor in-operando the effect of permanent magnets (B) on corrosion processes using metallic film (copper clad laminate), FeCl3 solution as corrosive medium, and digital camera to record the experiments. The results show that homogeneous and inhomogeneous B decrease or increase the corrosion rate, respectively. The homogeneous and inhomogeneous B also shows different corrosion patterns and induces rotation of the corrosive medium indicating the presence of the Lorentz force. The procedure proposed can also be applied to other metals and corrosive media providing valuable information on the corrosion process in the presence of B in several environmental conditions.

链接：https://www.nature.com/articles/s41529-022-00233-5

12. 标题：Ammonia synthesis by photocatalytic hydrogenation of a N2-derived molybdenum nitride

作者：Sangmin Kim, Yoonsu Park, Junho Kim, Tyler P. Pabst & Paul J. Chirik

摘要：Although metal complexes are known to split dinitrogen at ambient temperature and pressure, the synthesis of ammonia from these compounds with H2 as the terminal reductant is rarely achieved. Here we report a photocatalytic ammonia synthesis from a N2-derived terminal molybdenum nitride by using H2 as the terminal reductant. An iridium hydride photocatalyst mediates the reaction on irradiation with blue light. A molybdenum pentahydride was identified as the principal metal product to arise after ammonia release. Conversion of the molybdenum pentahydride back to the terminal molybdenum nitride was accomplished in three steps and completed a synthetic cycle for NH3 formation from N2 and H2. Mechanistic investigations support a pathway that involves photoexcitation of the iridium hydride and a subsequent energy

transfer rather than electron transfer. Deuterium labelling confirmed H2 as the source of the N–H bonds. This photodriven, proton-coupled electron transfer allows the use of H2 as the terminal reductant for the catalytic formation of NH3 from N2 using metal catalysts.

链接：https://www.nature.com/articles/s44160-022-00044-1

13. **标题：**Atomic-precision Pt6 nanoclusters for enhanced hydrogen electro-oxidation

作者：Xiaoning Wang, Lianming Zhao, Xuejin Li, Yong Liu, Yesheng Wang, Qiaofeng Yao, Jianping Xie, Qingzhong Xue, Zifeng Yan, Xun Yuan & Wei Xing

摘要：The discord between the insufficient abundance and the excellent electrocatalytic activity of Pt urgently requires its atomic-level engineering for minimal Pt dosage yet maximized electrocatalytic performance. Here we report the design of ultrasmall triphenylphosphine-stabilized Pt6 nanoclusters for electrocatalytic hydrogen oxidation reaction in alkaline solution. Benefiting from the self-optimized ligand effect and atomic-precision structure, the nanocluster electrocatalyst demonstrates a high mass activity, a high stability, and outperforms both Pt single atoms and Pt nanoparticle analogues, uncovering an unexpected size optimization principle for designing Pt electrocatalysts. Moreover, the nanocluster electrocatalyst delivers a high CO-tolerant ability that conventional Pt/C catalyst lacks. Theoretical calculations confirm that the enhanced electrocatalytic performance is attributable to the bifold effects of the triphenylphosphine ligand, which can not only tune the formation of atomically precise platinum nanoclusters, but also shift the d-band center of Pt atoms for favorable adsorption kinetics of *H, *OH, and CO.

链接：https://www.nature.com/articles/s41467-022-29276-7

14. **标题：** Limited solvation of an electron donating tryptophan stabilizes a photoinduced charge-separated state in plant (6–4) photolyase

作者： Yuhei Hosokawa, Pavel Müller, Hirotaka Kitoh-Nishioka, Shigenori Iwai & Junpei Yamamoto

摘要：(6–4) Photolyases ((6–4) PLs) are ubiquitous photoenzymes that use the energy of sunlight to catalyze the repair of carcinogenic UV-induced DNA lesions, pyrimidine(6–4)pyrimidone photoproducts. To repair DNA, (6–4) PLs must first undergo so-called photoactivation, in which their excited flavin adenine dinucleotide (FAD) cofactor is reduced in one or two steps to catalytically active FADH− via a chain of three or four conserved tryptophan residues, transiently forming FAD•−/FADH− ··· TrpH•+ pairs separated by distances of 15 to 20 Å. Photolyases and related photoreceptors cryptochromes use a plethora of tricks to prevent charge recombination of photoinduced donor–acceptor pairs, such as chain branching and elongation, rapid deprotonation of TrpH•+ or protonation of FAD•−. Here, we address Arabidopsis thaliana (6–4) PL (At64) photoactivation by combining molecular biology, in vivo survival assays, static and time-resolved spectroscopy and computational methods. We conclude that At64 photoactivation is astonishingly efficient compared to related proteins—due to two factors: exceptionally low losses of photoinduced radical pairs through ultrafast recombination and prevention of solvent access to the terminal Trp3H•+, which significantly extends its lifetime. We propose that a highly conserved histidine residue adjacent to the 3rd Trp plays a key role in Trp3H•+ stabilization.

链接：https://www.nature.com/articles/s41598-022-08928-0

15. **标题：** Quinoline based thiosemicarbazones as colorimetric chemosensors for fluoride and cyanide ions and DFT studies

作者： Rabia Basri, Nadeem Ahmed, Muhammad Khalid, Muhammad Usman Khan, Muhammad Abdullah, Asad Syed, Abdallah M. Elgorban, Salim S. Al-Rejaie, Ataualpa Albert Carmo Braga & Zahid Shafiq

摘要： High toxicity and extensive accessibility of fluoride and cyanide ions in diverse environmental media encouraged attention for scheming well-organized probes for their detection. Keeping in mind we have designed and synthesized thiosemicarbazone-based chemosensors RB-1, RB-2 and RB-3 for the detection of fluoride and cyanide ions. The structural elucidation of the synthesized chemosensors is done by employing different analytical techniques including nuclear magnetic resonance and electronic absorption specrtoscopies. Admirable detection limit, binding constant and fast response time (2 s) to F− and CN− ions enlarged the applications of these chemosensors. Additional confirmation of the sensing ability of these chemosensors is derived from DFT and TDDFT calculations with M06/6-311G(d,p) method by performing FMO, UV–Vis, QTAIM and global reactivity parameters elucidation. Overall results point out that investigated chemosensors are suitable candidates for sensing the F− ions. These chemosensors were successfully applied to detect F− ions in a commercial toothpaste sample.

链接： https://www.nature.com/articles/s41598-022-08860-3

16. **标 题 ：** Synthesis and characterization of highly efficient and recoverable Cu@MCM-41-(2-hydroxy-3-propoxypropyl) metformin mesoporous catalyst and its uses in Ullmann type reactions

作者： Zahra S. Robatjazi, M. Reza Naimi-Jamal & Mahdieh Tajbakhsh

摘要： The functionalized MCM-41-(2-hydroxy-3-propoxypropyl) metformin was prepared and anchored by copper ions to employ as a catalyst for the Ullmann C-X coupling reaction. The catalyst was characterized by Fourier-transform infrared spectroscopy, thermogravimetric analysis, X-ray diffraction, transmission electron microscopy, scanning electron microscopy, energy-dispersive X-ray spectroscopy measurements and, N2 adsorption–desorption isotherms. The benefits of this catalyst are the use of inexpensive and non-toxic metformin ligand, easy catalyst/product separation, and catalyst recycling. The catalyst can be reused at least for five repeated cycles without a significant loss of its catalytic activity or metal leaching

链接： https://www.nature.com/articles/s41598-022-08902-w

17. **标题：** Self-consistent determination of long-range electrostatics in neural network potentials

作者： Ang Gao & Richard C. Remsing

摘要： Machine learning has the potential to revolutionize the field of molecular simulation through the development of efficient and accurate models of interatomic interactions. Neural networks can model interactions with the accuracy of quantum mechanics-based calculations, but with a fraction of the cost, enabling simulations of large systems over long timescales. However, implicit in the construction of neural network potentials is an assumption of locality, wherein atomic arrangements on the nanometer-scale are used to learn interatomic interactions. Because of

this assumption, the resulting neural network models cannot describe long-range interactions that play critical roles in dielectric screening and chemical reactivity. Here, we address this issue by introducing the self-consistent field neural network — a general approach for learning the long-range response of molecular systems in neural network potentials that relies on a physically meaningful separation of the interatomic interactions — and demonstrate its utility by modeling liquid water with and without applied fields.

链接：https://www.nature.com/articles/s41467-022-29243-2

18. **标题：**Machine learning-assisted non-destructive plasticizer identification and quantification in historical PVC objects based on IR spectroscopy

作者：Tjaša Rijavec, David Ribar, Jernej Markelj, Matija Strlič & Irena Kralj Cigić

摘要：Non-destructive spectroscopic analysis combined with machine learning rapidly provides information on the identity and content of plasticizers in PVC objects of heritage value. For the first time, a large and diverse collection of more than 100 PVC objects in different degradation stages and of diverse chemical compositions was analysed by chromatographic and spectroscopic techniques to create a dataset used to construct classification and regression models. Accounting for this variety makes the model more robust and reliable for the analysis of objects in museum collections. Six different machine learning classification algorithms were compared to determine the algorithm with the highest classification accuracy of the most common plasticizers, based solely on the spectroscopic data. A classification model capable of the identification of di(2-ethylhexyl) phthalate, di(2-ethylhexyl) terephthalate, diisononyl phthalate, diisodecyl phthalate, a mixture of diisononyl phthalate and diisodecyl phthalate, and unplasticized PVC was constructed. Additionally, regression models for quantification of di(2-ethylhexyl) phthalate and di(2-ethylhexyl) terephthalate in PVC were built. This study of real-life objects demonstrates that classification and quantification of plasticizers in a general collection of degraded PVC objects is possible, providing valuable data to collection managers.

链接：https://www.nature.com/articles/s41598-022-08862-1

19. **标题：**Copper-doped functionalized β-cyclodextrin as an efficient green nanocatalyst for synthesis of 1,2,3-triazoles in water

作者：Mahdieh Tajbakhsh & Mohammad Reza Naimi-Jamal

摘要：The synthesis of 1,2,3-triazoles with immobilized Cu(I) in thiosemicarbazide-functionalized β-cyclodextrin (Cu@TSC-β-CD) as a supramolecular catalyst was discussed. The catalyst was characterized by Fourier-transform infrared spectroscopy (FT-IR), thermogravimetric analysis (TGA), X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS), and Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) measurements. The catalyst showed high activity (up to 95% yields of triazole products under optimized reaction conditions), providing a one-pot, atom-economic, and highly regioselective green method for 1,2,3-triazoles synthesis in an azide-alkyne cycloaddition (AAC) protocol in water. High stability and no appreciable leaching of Cu(I) were observed, owing to its strong binding via the coordination with thiosemicarbazide functionality.

链接：https://www.nature.com/articles/s41598-022-08868-9

20. **标题：**Boron clusters as broadband membrane carriers

作者：Andrea Barba-Bon, Giulia Salluce, Irene Lostalé-Seijo, Khaleel. I. Assaf, Andreas Hennig, Javier Montenegro & Werner M. Nau

摘要：The membrane translocation of hydrophilic substances constitutes a challenge for their application as therapeutic compounds and labelling probes1,2,3,4. To remedy this, charged amphiphilic molecules have been classically used as carriers3,5. However, such amphiphilic carriers may cause aggregation and non-specific membrane lysis6,7. Here we show that globular dodecaborate clusters, and prominently B12Br122−, can function as anionic inorganic membrane carriers for a broad range of hydrophilic cargo molecules (with molecular mass of 146–4,500 Da). We show that cationic and neutral peptides, amino acids, neurotransmitters, vitamins, antibiotics and drugs can be carried across liposomal membranes. Mechanistic transport studies reveal that the carrier activity is related to the superchaotropic nature of these cluster anions8,9,10,11,12. We demonstrate that B12Br122− affects cytosolic uptake of different small bioactive molecules, including the antineoplastic monomethyl auristatin F, the proteolysis targeting chimera dBET1 and the phalloidin toxin, which has been successfully delivered in living cells for cytoskeleton labelling. We anticipate the broad and distinct delivery spectrum of our superchaotropic carriers to be the starting point of conceptually distinct cell-biological, neurobiological, physiological and pharmaceutical studies.

链接：https://www.nature.com/articles/s41586-022-04413-w

IEL Top25

（来源：http://ieeexplore.ieee.org/）

1. **标题：**Fraction-of-Time Probability: Advancing Beyond the Need for Stationarity and Ergodicity Assumptions

出处：IEEE Access

作者：Antonio Napolitano; William A. Gardner

摘要：Time series arising from measurements in many fields of physics, engineering, chemistry, biology, and econometrics, are commonly modeled as sample paths from an ensemble which, together with a probability measure, is called a stochastic process. Stationarity and ergodicity assumptions about this model are generally made for analytical convenience and mathematical tractability of the model. In this article, it is shown that a dichotomy, which can be very misleading in practice, exists between the properties of a stochastic process and those of its individual sample paths. This dichotomy can be eliminated by adopting the fraction-of-time (FOT) probability approach reviewed in this article for which a probabilistic model is constructed from a single time series without introducing the abstraction of the stochastic process. Two FOT-probability models are reviewed. The first considers probabilistic functions that do not depend on time and employs the relative measure on the real line as a probability measure and the time average as an expectation operator. Such time series are called stationary signals. The second considers periodic, poly-periodic, and almost periodic probabilistic functions and employs the operator that extracts the finite-strength additive sine-wave components of its argument as an expectation operator. This latter model is appropriate for describing time series originating from phenomena involving a combination of periodic and random phenomena. Such time series are called cyclostationary, poly-cyclostationary, and almost cyclostationary signals. The FOT-probability alternative provides a means for circumventing two standard but undesirable practices: (1) Adopting the Kolmogorov stochastic process model by using its Axiom VI without being able to verify its validity for the specific application and (2) Assuming Birkhoff's ergodicity condition holds without being able to verify its validity for the specific application.

链接：https://ieeexplore.ieee.org/document/9743388

2. **标题：**MSFSA-GAN: Multi-scale fusion self attention generative adversarial network for single image deraining

出处：IEEE Access

作者：Wang Xue; Cheng Huan-xin; Sun Sheng-yi; Jiang Ze-qin; Cheng Kai; Cheng Li

摘要：Bad weather such as rainy days will seriously affect the image quality and the accuracy of visual processing algorithm. In order to improve the image deraining quality, a multi-scale fusion self attention generation adversarial network (MSFSA-GAN) is proposed. This network uses different scales to extract input characteristics of rain lines. First, Gaussian pyramid rain maps

with different scales are generated by Gaussian algorithm. Then, in order to extract the features of rain lines with different scales, the coarse fusion module and fine fusion module are designed respectively. Next, the extracted features are fused at different scales. In this process, the self attention mechanism is introduced to make the network focus on the extracted features of different scales. And before the fusion, the rain pattern reconstruction operation is also carried out, so that the network can reproduce the input image more perfectly. Finally, it is input into the discriminator network with dense blocks to obtain the image that removes the rain lines. We used R100H and R100L datasets to train and test our network. The results show that our method as high as 27.79 in PSNR and UQI is 0.94, which is superior to the existing methods in performance. Meanwhile, we also compared the cost of time, the result of our network is only 0.02s.

链接：https://ieeexplore.ieee.org/document/9741786

3. **标题：**Generation of a flat-top magnetic field with multiple-capacitor power supply

出处：IEEE Access

作者：Dake Li; Hongfa Ding; Yuchao Fang; Song Zhang; Daiyuan Pan

摘 要： The flat-top magnetic field (FTMF) can meet scientific experimental requirements for higher magnetic intensity, longer flat-top pulse width, and lower ripple in physics, chemistry, biology, and other scientific fields. This paper proposes an FTMF system powered by the multiple-capacitor power supply (MCPS). The MCPS consists of several capacitor banks with customizable capacitance and given voltage. These banks discharge sequentially based on the designed time-series to yield an FTMF. Compared with other methods for generating the FTMF, the MCPS can easily generate FTMFs with high parameters and flexible adjustability of the pulse width. Due to the coupled variable parameters between and within the power supply and the magnet, a hybrid algorithm based on the genetic algorithm (GA) and particle swarm optimization (PSO) is applied to calculate the discharge parameters of the MCPS. The optimal solution from the GA-PSO hybrid algorithm is visualized and selected by the basis vector method. For verifying the effectiveness of the MCPS and the optimization method, a series of FTMFs at different magnetic field strength levels are modeled in MATLAB/Simulink and achieved in the experiment. The generated FTMF with the highest field strength is 50 T, its pulse width is 70 ms, and ripple is less than 0.7%.

链接：https://ieeexplore.ieee.org/document/9741708

4. **标题：**Autonomy and perseverance in a blended learning Case of ESTEEM program "Energizing STEM Teachers through English Exploration in Morocco"

出处：2022 2nd International Conference on Innovative Research in Applied Science, Engineering and Technology (IRASET)

作者：Abdessamad El Omari; Said Lamrabat; Malika Tridane; Said Belaaouad

摘要： Persistence in distance learning is a major issue and challenge for learners as well as for training designers and organizations. It be caused by social, emotional, technical, cognitive, or metacognitive reasons. Addressing these individual factors that motivate learners to continue or to drop out is at the heart of cognitive theories. This paper is a mixed-methods study that attempts to examine the phenomenon of persistence and its correlation with learning practices implemented in distance learning. Learners in the ESTEEM program "Energizing Science Technology

Engineering Mathematics Teachers Through English Exploration in Morocco" constitute the sample of this case study. The purpose of this study is to understand to what extent the motivational profile of learners can influence the success of a blended learning? And what impact autonomy has on the learner's decision to persist or to drop out of a blended learning experience? The results show that most learners who have completed the course have a high degree of autonomy. Learners must then develop this skill. The e-learning devices designers and trainers must also support the development of this skill by learners in order to make e-learning programs successful.

链接：https://ieeexplore.ieee.org/document/9738065

5. **标题：**Performance improvement of a TEG by a heat transfer fluid

出处：2022 2nd International Conference on Innovative Research in Applied Science, Engineering and Technology (IRASET)

作者：Sara Jennah; Naoual Belouaggadia; Rachid Lbibb; Mohammed Ezzine

摘 要： This This paper presents an optimization method to improve the performance of thermoelectric modules by managing their operating conditions. The studied mechanism, corresponding to an original configuration of the thermoelectric heat pump, includes thermocouples with channels in which water circulates in contact with both sides of the TEMs. The objective function is to regulate the temperature of the cold welds. In the first instance, a hot heat transfer fluid will flow through the thermopile at the hot welds, and then a cold heat transfer fluid will flow through the cold welds. The results obtained show that when the cold heat transfer fluid is added, better efficiency is obtained, and this is due to the remarkable temperature difference obtained.

链接：https://ieeexplore.ieee.org/document/9738018

6. **标题：**A simulation study of the impact of the COVID-19 crisis on the energy demand of a building located in a semi-arid climate in Morocco

出处：2022 2nd International Conference on Innovative Research in Applied Science, Engineering and Technology (IRASET)

作 者： Salma Ouhaibi; Omar Iken; Naoual Belouaggadia; Mohammed Ezzine; Rachid Lbibb; Miloud Rahmoune

摘要：The COVID-19 epidemic increases the uncertainty of energy demand. This paper aims to study the impact of containment measures due to the COVID-19 epidemic on the energy demand of a group of buildings in a neighborhood and evaluate the different techniques studied on thermal performance and energy savings. Indeed, this study shows the importance of using natural and recycled waste-based materials and nighttime radiative cooling during the summer period. For this purpose, a full-scale cell located in Casablanca was considered a case study to build a simulation model performed on TRNSYS, validated using the experimental results. This model is then used to impact the techniques studied on energy performance and hours of discomfort inside another cell in Marrakech. As a result, this study has shown that the passive techniques integrated into the cell, using the material based on sisal/wool nonwoven, and night-time radiative cooling during summer, reduce energy requirements compared to the reference configuration.

链接：https://ieeexplore.ieee.org/document/9737916

7. **标题：**Characterization of a new clay site in the context of valorization in the construction sector

出处：2022 2nd International Conference on Innovative Research in Applied Science, Engineering and Technology (IRASET)

作 者 ： Boutaina Moumni; Hayat Benmoussa; Abdallah Oulmekki; Dolores Eliche Quesada; Mohammed Charrou

摘要：A site in the Missour region that has never been exploited before has been subjected to a physical and chemical characterization in order to understand its mineralogical composition and to determine if it can be used in the construction sector. Different analyses were carried out such as X-Ray diffraction (XRD), X-ray Fluorescence (XRF), Thermal behavior analysis (DTG-TG), Infrared spectroscopy (IR), Granulometry laser analysis, Scanning Electron Microscope and Energy Dispersive X-ray Spectroscopy (SEM-EDXS) indicating the presence of Illite, Quartz, and Calcite as minerals which constitute this material.

链接：https://ieeexplore.ieee.org/document/9738051

8. **标题：**The Contact Angle of Cellulosic Materials: Transforming Natural Dyes into Biomaterials for Sustainability and Green Energy

出处：2022 2nd International Conference on Innovative Research in Applied Science, Engineering and Technology (IRASET)

作者：Sara Rbihi; Latifa Laallam; Ahmed Jouaiti

摘要：This research provides an insight into the contact angle and diffusion of natural dyes into cellulosic materials, while taking into account the structure and compositional effect of the cellulosic surface. The contact angle determination was based on an experimental device using software to analyze images and measure the contact angles by calculating the tangent of the profile. Results show that dye contact angle depends on the type of cellulosic material and the type of dye. The rate of dye contact angle decreases when the structure of matrial is more amorphous. Decreasing the crystallinity rate provides the increase in cross-linking and grain boundaries on the surface, which improves the diffusion of dye into the weave. This approach makes it possible to develop highly hydrophilic or hydrophobic surface tissues while studying the crystallinity of the cellulosic source. The cost, ease and environmental friendliness of these dyes are the main reasons for the increased interest in developing this type of dyes.

链接：https://ieeexplore.ieee.org/document/9737753

9. **标题：**Study of Conversion of Peanut Hulls to Solid Biofuel

出处：2022 2nd International Conference on Innovative Research in Applied Science, Engineering and Technology

作者：Hadey Chaimaa; Loulidi Ilyasse; Boukhlifi Fatima; Kali Abderrahim; Jabri Maria; Alami Mohamed;

摘要：The shortage of oil and the ever-increasing pollution are forcing countries to diversify their means of energy production and in particular to think of renewable energies. In this study we are interested in the production of solid biofuel from peanut shells by heat treatment. The study of the combustion properties using thermogravimetric analysis under oxidizing atmosphere showed us

that the combustion behavior of the raw biomass differs from its biochar, compared to its raw biomass, the biochar has good characteristics of combustion and high energy content. The calorific value has increased significantly from 12 to 21 which offers the biochar important combustion properties.

链接：https://ieeexplore.ieee.org/document/9738303

10. **标题：**Effect of Carrier gas on sensitivity of Surface Acoustic Wave Detector

出处：IEEE Sensors Journal

作者：Jitender Kumar; A.T. Nimal; Upendra Mittal; Vinod Kumar; Vinay Kumar Singh

摘要：Enhancement of sensitivity is a hot pursuit for every kind of sensor/detector. While many methods are exploited for various sensors/detectors for this, the methods are specific in nature for the technology involved. This article discusses a novel study where enhancement of sensitivity, specific to a Surface Acoustic Wave (SAW) device used as a Gas Chromatographic (GC) detector is achieved by using a proper carrier gas. With an ultimate aim of implementing the outcome on SAW-GC based, handheld, Chemical Warfare Agent (CWA) Electronic-Nose vapour detector being developed at our laboratory, four different carrier gases i.e. Hydrogen, Helium, Nitrogen and Zero air were subjected to the scrutiny for its impact on sensitivity. Detection of a CWA simulant, 2-Chloro-Ethyl-Ethyl-Sulfide (CEES), 1,5-Dichloropentane (DCP) simulating Sulphur Mustard (H Agent), Di-methylmethyl phosphonate (DMMP), Diethyl cyanophosphonate (DECP), Triethyl pohosphate (TEP) simulating G-Agents along with three Volatile Organic Compounds (VOCs) i.e. Methanol, Toluene and Xylene were carried out in the study. A fast-GC with 70 seconds chromatogram, with appropriate GC parameters is used for the study in order to cater for the handheld battery operated rapid detector. A spread of more than two times in sensitivity could be seen while using common GC carrier gases in the range of concentration (200-2000ppm) studied. By virtue of GC with SAW detector, excellent selectivity, repeatability, and long term stability is achieved. A detailed discussion on the reasons for the same is presented.

链接：https://ieeexplore.ieee.org/document/9740674

11. **标题：**Real-time State of Charge Estimation of Lithium-ion Batteries Using Optimized Random Forest Regression Algorithm

出处：IEEE Transactions on Intelligent Vehicles

作者：M S Hossain Lipu; M A Hannan; Aini Hussaion; Shaheer Shaheer Ansari; S A Rahman; Mohamad H.M.

摘要：Abstract-This paper presents an improved machine learning approach for the accurate and robust state of charge (SOC) in electric vehicle (EV) batteries using differential search optimized random forest regression (RFR) algorithm. The precise SOC estimation confirms the safety and reliability of EV. Nevertheless, SOC is influenced by numerous factors which cannot be measured directly. RFR is suitable for real-time SOC estimation due to its robustness to noise, overfitting issues and capacity to work with huge datasets. However, proper selection of RFR architecture and hyper-parameters combination remains a key issue to be explored. Hence, a differential search algorithm (DSA) is employed to search for the optimal values of trees and leaves in the RFR algorithm. DSA optimized RFR eliminates the utilization of the filter in data pre-processing steps and does not require a detailed understanding and knowledge about battery chemistry, rather only

needs sensors to monitor battery voltage and current. The developed approach is validated at room temperature using two types of lithium-ion batteries under a pulse discharge test. In addition, the proposed model is verified under varying temperature settings under EV drive cycles. The experimental results demonstrate that the DSA optimized RFR algorithm achieves RMSE of 0.382% in the HPPC test using LiNMC battery. Besides, the proposed method obtains satisfactory outcomes in EV drive cycles, estimating MAE of 0.193% and 0.346% in DST and FUDS cycles, respectively, at 25°C.

链接：https://ieeexplore.ieee.org/document/9740509

12. **标题：**Compressed computational ghost imaging based on array sampling

出 处 ： 2022 IEEE 6th Information Technology and Mechatronics Engineering Conference (ITOEC)

作者：Xuan Liu; Tengyuan Gao; Jigui Mao; Tailin Han; Cheng Zhou; Mingchi Ju; Bo Xu; Lijun Song

摘要：Computational ghost imaging as a new imaging method, has attached the interest of many researchers. However, the practical application of computational ghost imaging is limited by the slow imaging speed of computational ghost imaging and the low quality of reconstructed images. Therefore, this paper proposes a compressed computational ghost imaging method based on array sampling, which uses the array detector to significantly increase the imaging speed of computational ghost imaging and achieve high-quality image reconstruction under low sampling times with compressed sensing. The experimental results show that the imaging method proposed in this paper achieves a speed increase of more than 4 times compared with single-pixel computing ghost imaging. Even at the sampling rate of 1.8%, high quality reconstructed images can still be obtained. Therefore, the method can promote the application of computational ghost imaging in real-time imaging, real-time detection and other fields.

链接：https://ieeexplore.ieee.org/document/9734689

13. **标题：**Optical Diagnostics of Plasma Assisted Chemical Looping Reactions

出处：IEEE Transactions on Plasma Science

作者：Rajagopalan V. Ranganathan; Shaon Talukdar; Mruthunjaya Uddi

摘 要 ： Here, we study time- and spatially resolved heterogeneous plasma catalysis chemical looping reactions using in situ laser diagnostics in a novel parallel plate dielectric barrier discharge (DBD) plasma reactor at atmospheric pressure and temperatures: 473 and 673 K. A chemical looping material, 50:50 by mass mixture of lanthanum-nickel-based perovskite (La 0.9 Ce 0.1 NiO_3) and CeO_2 , was placed directly in non-equilibrium DBD plasma. Optical diagnostic techniques used include high-speed imaging (i.e., ns gate width), N_2 optical emission spectroscopy (OES) at 337 nm, and Rayleigh scattering (RS). During the reduction step, a mixture of CH_4 , CO_2 , and N_2 flow was used, and during the oxidation step, the airflow was used. During the reduction step, the average temperatures measured at the furnace setpoint temperature of 473 and 673 K were 580 and 800 K, respectively. For the oxidation step, the average temperatures measured were 520 and 830 K, respectively. There was good agreement in average temperatures measured by RS and N_2 OES. The 2-D RS imaging showed lower temperatures near the catalyst during the reduction step and higher temperatures during the oxidation step.

Although corona discharges were observed over chemical looping materials in high-speed images, RS temperature measurements showed non-equilibrium plasma chemistry over the materials.
链接：https://ieeexplore.ieee.org/document/9740018

14. **标题：**Highly proton conductive membranes based on lignin/ZrP/PTFE composite for high temperature PEM fuel cells
出处：2022 Advances in Science and Engineering Technology International Conferences (ASET)
作 者： Muhammad Tawalbeh; Amani Al-Othman; Ahmad Ka'ki; Afifa Farooq; Malek Alkasrawi
摘要：Novel lignin/zirconium phosphate (ZrP) based membranes for proton exchange membrane fuel cells applications were synthesized and studied in this work. The effects of lignin along with other additives such as ionic liquids and glycerol were investigated in terms of proton conductivity. Lignin was found to enhance the proton conductivity of pure ZrP membranes by one order of magnitude from 0.1 to 1 mS/cm. The addition of glycerol to the lignin/zirconium phosphate enhanced the proton conductivity with the highest value to be 20.2 mS/cm at 1.0 %wt. glycerol. Among three different ionic liquids that were investigated in this work, the highest proton conductivity was obtained with 1-Hexyl-3-methylimidazolium tricyanomethanide [HMIM][C 4 N 3 -] ionic liquid at 0.3 %wt. The addition of [HMIM][C 4 N 3 -] to the lignin/ZrP based membranes gave a proton conductivity of 100 mS/cm.
链接：https://ieeexplore.ieee.org/document/9734834

15. **标题：**The effect of feed temperature and pressure on the performance of single stage reverse osmosis desalination system
出处：2022 Advances in Science and Engineering Technology International Conferences (ASET)
作 者： Abdulaziz Fares Naji Moqbel; Abdulwehab Adem Ibahim; Azmi Alazzam; Ghassan Malkawi;
摘 要：Reverse osmosis is a technology that is used to eliminate a variety of impurities from seawater or brackish water by using pressure to force the water molecules into the membrane. In this study, an Aspen Plus platform which is integrated with an Excel spreadsheet, is used to build a single stage reverse osmosis of spiral wound membrane. This work aims to investigate the performance of spiral wound membranes as a factor of feed temperature and pressure. Some of the outcomes obtained due to the impact of feed pressure, like the salt rejection, incrementally increased from 99.7% to 99.94%, and the permeate flow rate reached 43.6% from the total feed inlet.
链接：https://ieeexplore.ieee.org/document/9734963

16. **标题：**Electrical and Optical Characterisation of CZTS Thin-Film for Sensing Applications
出处：2022 Advances in Science and Engineering Technology International Conferences (ASET)
作者：Atul Kumar; Narender Kumar; Pranay Ranjan; Ajay D Thakur
摘要：The low-cost, earth abundant kesterite copper-zinc-tin-sulfide (CZTS) is the most desirable material for the upcoming sustainable energy, sensors and energy storage as well as generation. However, the research on the material was hindered due to the instability of the zinc and copper in the quaternary phase, thus, resulting in secondary complex phase with defects. This led to the

structural inhomogeneity, challenges in the repeatability of the synthesis procedure and degradation (especially) in the efficiency of the solar cell. Therefore, synthesis of CZTS in right phase and purity (without any stoichiometric imbalance as well as secondary phases and defects) is a challenge to overcome. Moreover, due to the presence of copper and zinc, it is an interesting material for the scientific community as gas sensor. In this report we have synthesized CZTS through chemical synthesis and examined a spin coated CZTS thin film for probable sensing application at room temperature. We utilized the CZTS thin-film for room temperature gas sensing of the volatile organic compound (ethanol) at 68 PPM. In addition, the Phase purity of the film was confirmed by the X-ray diffraction. While, the optical characterization of the film was investigated by the UV-Spectrometer. Thickness of the film was confirmed by atomic force microscopy and the electrical characterization of the film was done by Kiethley 2420.
链接：https://ieeexplore.ieee.org/document/9734877

17. **标题：**Hydro Power Production in Jordan: Possibilities and Challenges
出处：2022 Advances in Science and Engineering Technology International Conferences (ASET)
作者：Diala Siam; Malek Alkasrawi; Emad Abdelsalam; Tareq Salameh; Hamzah Nawafah;
摘要：Jordan has limited energy resources combined with an increasing population over the past 20 years. There are limited resources such as fossil fuels and natural gas. Therefore, Jordan relies on imports of crude oil and natural gas. Jordan has several water reservoirs in the form of a dam that spread all over the country. No of these dams are utilized for hydropower production. In this work, we identified the dams that are potentially could be modified for energy production. We estimated the overall power production with recommendations and present and future challenges.
链接：https://ieeexplore.ieee.org/document/9734862

18. **标题：**Investigation of Atomic Layer Futuristic Memory Devices of Binary Chalcogenides WX2 (X = S and Se): First-Principles Study
出处：2022 Advances in Science and Engineering Technology International Conferences (ASET)
作者：Narender Kumar; Na'il Saleh; Arun Kumar; Mohan Lal Verma; Pranay Ranjan
摘要：We have investigated the spin-dependent structural, electronic and localized-induced magnetic moment in an atomic layer of binary chalcogenide semiconductors, Tungsten sulphide/selenide (WX 2 , where X= S, Se) using first-principle calculations. It was observed that the addition of fluorine to the WX 2 monolayer lattice reduces the bandgap of the material and induced a magnetic moment of ~1 Bohr magneton. Moreover, the reasons behind this magnetic transition from non-magnetic semiconductors to magnetic semiconductors were investigated and discussed. The calculated binding energy reveals that the pristine monolayer is more stable than the fluorine doped WX 2 sheet. Also, intermittent energy levels were created due to the fluorine atoms and resulted in p-type acceptor semiconductor behaviour in spin up and n-type donor behaviour in spin-down of WX 2 monolayer. It was observed that the unparalleled behaviour of spin can be tuned to suitable applications such as memory devices and spintronics.
链接：https://ieeexplore.ieee.org/document/9735000

19. **标题：**Passivation of Perovskite Films Using Ionic Liquids
出处：2022 Advances in Science and Engineering Technology International Conferences (ASET)

作者：Adnan Alashkar; Taleb Ibrahim; Mustafa Khamis; Abdul Hai Alami

摘要：In this paper, the carrier recombination, and dynamics of Perovskite Solar Cells (PSC) are investigated. Ionic Liquids (IL) are presented in the bulk perovskite in an attempt to improve the dynamics of the charge transport layer. Time Resolved Photoluminescence (TRPL) is utilized to study the fast electronic decay of the perovskite samples and the influence of the IL on the stability of the perovskite film. The ILs are added to the perovskite in three ratios (5%, 10%, and 20%). The results showed that the presence of the ILs increases the electron lifetime inside the perovskite layer. In addition, 10% IL/perovskite displayed the highest increase of 72% in the lifetime. Where, for higher ratios, the lifetime started deteriorating.

链接：https://ieeexplore.ieee.org/document/9734860

20. 标题：Concentrated Solar Power: Technology and Potential in Jordan

作者：Omar Al Farah; Malek Alkasrawi; Emad Abdelsalam; Tareq Salameh; Mohammad Al-Shannag

出处：2022 Advances in Science and Engineering Technology International Conferences (ASET)

摘要：As energy demands increases year by year, we must find sources of energy that compensate for the increased demand while at the same time limiting our use of conventional sources of energy since their available resources are dwindling yearly, and because of their harmful effect on the environment and their part in increasing the effects of climate change. This means the share of renewables in the energy share mix must increase. A great method of generating renewable energy is the use of Concentrated Solar Power (CSP), which generally operates on a Rankine cycle for generating energy, by concentrating sun rays using reflectors at a point, or along several points, which contain the working fluid of the cycle. The working fluid is then heated by the reflected solar energy due to solar thermal energy and is used to generate steam that is fed into the Rankine cycle to eventually generate electricity. CSP plants however are not a 100% fully renewable sources of energy as some plants substitute differences in production using fossil fuels, and some CSP plants can be combined with already existing conventional power plants. CSP also has a great advantage against other renewable sources since it can be dispatchable using a thermal storage that stores heat and allows it to keep generating electricity for some time when there is no sunlight.CSP is still relatively an expensive form of renewable energy, however in recent years its costs are steadily dropping, with investments and new projects increasing, with Spain being the country with the most CSP plants globally. Jordan has introduced a few plans for CSP plants to be built in the southern region of Jordan, given its high potential for generating electricity using this method.

链接：https://ieeexplore.ieee.org/document/9735097

21. 标题：Superhydrophobic Fluorosilane and Alkylsilane Diatomaceous Earth Particles Treated Polyurethane

出处：2022 Advances in Science and Engineering Technology International Conferences (ASET)

作者：Helanka J. Perera; Frank D. Blum

摘要：Hydrophobic and superhydrophobic coatings were prepared using fluorosilane (FS) and alkylsilane (AS) modified diatomaceous earth (DE) with a polyurethane. The thermal properties of

modified FS-DE and AS-DE were probed using thermogravimetric analysis yielding 3.8% and 6.8% silane adsorption, respectively. The hydrophilicity and morphology of the materials were analyzed using contact angles and scanning electron microscopy. The water contact angles were studied as a function of the particle loadings of fluorosilane and alkylsilane modified DE in the coatings. The water contact angles reached superhydrophobicity (water contact angles ≥ 150°) with 20% and 30% particle loadings of FS-DE and AS-DE, respectively. For FS-DE, the contact angle reached 160° with more than 20% particle loadings, while AS-DE remained superhydrophobic between 30-50% particle loadings. Above 50% AS-DE particle loadings, the contact angles were reduced. These results were consistent with those from scanning electron microscopy.

链接：https://ieeexplore.ieee.org/document/9735078

22. **标题：**The Soft Compiler: A Web-Based Tool for the Design of Modular Pneumatic Circuits for Soft Robots

出处：IEEE Robotics and Automation Letters

作者：Savita Vitthalrao Kendre; Lauryn Whiteside; Tian Yu Fan; Jovanna Tracz; Gus Teran;

摘要：Developing soft circuits from individual soft logic gates poses a unique challenge: with increasing numbers of logic gates, the design and implementation of circuits lead to inefficiencies due to mathematically unoptimized circuits and wiring mistakes during assembly. It is therefore practically important to introduce design tools that support the development of soft circuits. We developed a web-based graphical user interface, the Soft Compiler, that accepts a user-defined robot behavior as a truth table to generate a mathematically optimized circuit diagram that guides the assembly of a soft fluidic circuit. We describe the design and experimental verification of three soft circuits of increasing complexity, using the Soft Compiler as a design tool and a novel pneumatic glove as an input interface. In one example, we reduce the size of a soft circuit from the original 11 logic gates to 4 logic gates while maintaining circuit functionality. The Soft Compiler is a web-based design tool for fluidic, soft circuits and published under an open-source MIT License.

链接：https://ieeexplore.ieee.org/document/9736571

23. **标题：**Pectin-coated baclofen-layered zinc hydroxide nanohybrid as a bio-based nanocomposite carrier for the oral delivery

出处：IEEE Transactions on NanoBioscience

作者：Hafezeh Nabipour; Sadia Batool; Yuan Hu

摘要：pH-sensitive pectin beads were proposed as a protective capsule for layered zinc hydroxide-drug (LZH-Drug) nanohybrids in the gastrointestinal tract in this paper. Baclofen was intercalated between LZH layers using the co-precipitation method as a model drug. By combining LZH-baclofen with pectin, the resulting nanohybrid (LZH-baclofen) was used to make bio-nanocomposite hydrogel beads. FTIR, XRD, and SEM analyses were used to characterize the produced products. Baclofen anions are vertical to the LZH layers in the shape of a monolayer, according to the interlayer space of 19.6 Å. The presence of nanocomposites is demonstrated by FTIR, which exhibits a peak at 3489 cm-1 for the OH group, 1564 and 1384 cm-1 for the –COO-vibration mode, indicating that baclofen is intercalated between the layered structures.

After intercalation, baclofen's thermal stability is greatly improved. The nanohybrid is more compact, with agglomerates and flat surfaces of the intercalated substance, shown by SEM. In vitro release behaviors of baclofen from LZH and bio-nanocomposites in buffer solution were examined under pH values (pH=1.2, 6.8, 7.4) chosen from a model of the passing materials through the gastrointestinal tract. For pectin encapsulated LZH-baclofen nanohybrid, drug release studies indicated superior protection against stomach pH and regulated release under intestinal tract conditions. Furthermore, nanohybrid and nanocomposite treatment of a normal fibroblast cell line resulted in cell survival up to 12.5 g/mL for a 24-h period, with inhibition reducing dose-dependently at higher concentrations. A novel intercalation molecule with a sustained release mode and improved toxicity against normal fibroblast cell lines has been produced as a result of the strong host-guest contacts between the LZH lattice and the baclofen anion. Further study into the utilization of brucite-like host materials in drug delivery systems should be based on these findings.

链接：https://ieeexplore.ieee.org/document/9737011

24. **标题：**Toward Delicate Anomaly Detection of Energy Consumption for Buildings: Enhance the Performance From Two Levels

出处：IEEE Access

作者：Dong Wang; Therese Enlund; Johan Trygg; Mats Tysklind; Lili Jiang

摘 要： Buildings are highly energy-consuming and therefore are largely accountable for environmental degradation. Detecting anomalous energy consumption is one of the effective ways to reduce energy consumption. Besides, it can contribute to the safety and robustness of building systems since anomalies in the energy data are usually the reflection of malfunctions in building systems. As the most flexible and applicable type of anomaly detection approach, unsupervised anomaly detection has been implemented in several studies for building energy data. However, no studies have investigated the joint influence of data structures and algorithms' mechanisms on the performance of unsupervised anomaly detection for building energy data. Thus, we put forward a novel workflow based on two levels, data structure level and algorithm mechanism level, to effectively detect the imperceptible anomalies in the energy consumption profiles of buildings. The proposed workflow was implemented in a case study for identifying the anomalies in three real-world energy consumption datasets from two types of commercial buildings. Two aims were achieved through the case study. First, it precisely detected the contextual anomalies concealed beneath the time variation of the energy consumption profiles of the three buildings. The performance in terms of areas under the precision-recall curves (AUC_PR) for the three given datasets were 0.989, 0.941, and 0.957, respectively. Second, more broadly, the joint effect of the two levels was examined. On the data level, all four detectors on the contextualized data were superior to their counterparts on the original data. On the algorithm level, there was a consistent ranking of detectors regarding their detecting performances on the contextualized data. The consistent ranking suggests that local approaches outperform global approaches in the scenarios where the goal is to detect the instances deviating from their contextual neighbors rather than the rest of the entire data.

链接：https://ieeexplore.ieee.org/document/9737138

25. **标题：**The State of Fortran

出处：Computing in Science & Engineering

作者：Laurence Kedward; Balint Aradi; Ondrej Certik; Milan Curcic; Sebastian Ehlert; Philipp Engel

摘要：A community of developers has formed to modernize the Fortran ecosystem. In this article, we describe the high-level features of Fortran that continue to make it a good choice for scientists and engineers in the 21st century. Ongoing efforts include the development of a Fortran standard library and package manager, the fostering of a friendly and welcoming online community, improved compiler support, and language feature development. The lessons learned are common across contemporary programming languages and help reduce the learning curve and increase adoption of Fortran.

链接：https://ieeexplore.ieee.org/document/9736688

ESI HOT PAPERS

(Chemistry)

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

1 被引频次：23487
题目：ELECTROCHEMICAL PHOTOLYSIS OF WATER AT A SEMICONDUCTOR ELECTRODE
作者：FUJISHIMA, A (FUJISHIMA, A); HONDA, K (HONDA, K)
出处：NATURE
摘要：ALTHOUGH the possibility of water photolysis has been investigated by many workers, a useful method has only now been developed. Because water is transparent to visible light it cannot be decomposed directly, but only by radiation with wavelengths shorter than 190 nm (ref. 1).

2 被引频次：16302
题目：Two-dimensional gas of massless Dirac fermions in graphene
作者：Novoselov, KS (Novoselov, KS); Geim, AK (Geim, AK); Morozov, SV (Morozov, SV); Jiang, D (Jiang, D); Katsnelson, MI (Katsnelson, MI); Grigorieva, IV (Grigorieva, IV); Dubonos, SV (Dubonos, SV); Firsov, AA (Firsov, AA)
出处：NATURE
摘要：Quantum electrodynamics (resulting from the merger of quantum mechanics and relativity theory) has provided a clear understanding of phenomena ranging from particle physics to cosmology and from astrophysics to quantum chemistry(1-3). The ideas underlying quantum electrodynamics also influence the theory of condensed matter(4,5), but quantum relativistic effects are usually minute in the known experimental systems that can be described accurately by the non-relativistic Schrodinger equation. Here we report an experimental study of a condensed-matter system (graphene, a single atomic layer of carbon(6,7)) in which electron transport is essentially governed by Dirac's (relativistic) equation. The charge carriers in graphene mimic relativistic particles with zero rest mass and have an effective 'speed of light' c* approximate to 10(6) m s(-1). Our study reveals a variety of unusual phenomena that are characteristic of two-dimensional Dirac fermions. In particular we have observed the following: first, graphene's conductivity never falls below a minimum value corresponding to the quantum unit of conductance, even when concentrations of charge carriers tend to zero; second, the integer quantum Hall effect in graphene is anomalous in that it occurs at half-integer filling factors; and third, the cyclotron mass m(c) of massless carriers in graphene is described by E = m(c)c(*)(2). This two-dimensional system is not only interesting in itself but also allows access to the subtle and rich physics of quantum electrodynamics in a bench-top experiment.
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3 被引频次：13519
题目：Building better batteries
作者：Armand, M (Armand, M.); Tarascon, JM (Tarascon, J. -M.)
出处：NATURE
摘要：The technological revolution of the past few centuries has been fuelled mainly by variations of the combustion reaction, the fire that marked the dawn of humanity. But this has come at a price: the resulting emissions of carbon dioxide have driven global climate change. For the sake of future generations, we urgently need to reconsider how we use energy in everything from barbecues to jet aeroplanes and power stations.
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4 被引频次：12386
题目：Materials for electrochemical capacitors
作者：Simon, P (Simon, Patrice); Gogotsi, Y (Gogotsi, Yury)
出处：NATURE MATERIALS
摘要：Electrochemical capacitors, also called supercapacitors, store energy using either ion adsorption (electrochemical double layer capacitors) or fast surface redox reactions (pseudo-capacitors). They can complement or replace batteries in electrical energy storage and harvesting applications, when high power delivery or uptake is needed. A notable improvement in performance has been achieved through recent advances in understanding charge storage mechanisms and the development of advanced nanostructured materials. The discovery that ion desolvation occurs in pores smaller than the solvated ions has led to higher capacitance for electrochemical double layer capacitors using carbon electrodes with subnanometre pores, and opened the door to designing high-energy density devices using a variety of electrolytes. Combination of pseudo-capacitive nanomaterials, including oxides, nitrides and polymers, with the latest generation of nanostructured lithium electrodes has brought the energy density of electrochemical capacitors closer to that of batteries. The use of carbon nanotubes has further advanced micro-electrochemical capacitors, enabling flexible and adaptable devices to be made. Mathematical modelling and simulation will be the key to success in designing tomorrow's high-energy and high-power devices.
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5 被引频次： 11208
题目：Synthesis of graphene-based nanosheets via chemical reduction of exfoliated graphite oxid
作 者： Stankovich, S (Stankovich, Sasha); Dikin, DA (Dikin, Dmitriy A.); Piner, RD (Piner, Richard D.); Kohlhaas, KA (Kohlhaas, Kevin A.); Kleinhammes, A (Kleinhammes, Alfred); Jia, Y (Jia, Yuanyuan); Wu, Y (Wu, Yue); Nguyen, ST (Nguyen, SonBinh T.); Ruoff, RS (Ruoff, Rodney S.)
出处：CARBON
摘 要： Reduction of a colloidal suspension of exfoliated graphene oxide sheets in water with hydrazine hydrate results in their aggregation and subsequent formation of a high-surface-area carbon material which consists of thin graphene-based sheets. The reduced material was characterized by elemental analysis, thermo-gravimetric analysis, scanning electron microscopy, X-ray photoelectron spectroscopy, NMR spectroscopy, Raman spectroscopy, and by electrical conductivity measurements. (c) 2007 Elsevier Ltd. All rights reserved.
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6 被引频次：11009
题目： Gold nanoparticles: Assembly, supramolecular chemistry, quantum-size-related properties, and applications toward biology, catalysis, and nanotechnology
作者：Daniel, MC (Daniel, MC); Astruc, D (Astruc, D)
出处：CHEMICAL REVIEWS
地址： Univ Bordeaux 1, LCOO, UMR CNRS 5802, Mol Nanosci & Catalysis Grp, F-33405 Talence, France.

7 被引频次：10685
题目：Visible-light photocatalysis in nitrogen-doped titanium oxides
作者：Asahi, R (Asahi, R); Morikawa, T (Morikawa, T); Ohwaki, T (Ohwaki, T); Aoki, K (Aoki, K); Taga, Y (Taga, Y)
出处：SCIENCE
摘要：To use solar irradiation or interior Lighting efficiently, we sought a photocatalyst with high reactivity under visible Light. Films and powders of TiO2-XNX have revealed an improvement over titanium dioxide (TiO2) under visible Light (wavelength < 500 nanometers) in optical absorption and photocatalytic activity such as photodegradations of methylene blue and gaseous acetaldehyde and hydrophilicity of the film surface, Nitrogen doped into substitutional sites of TiO2 has proven to be indispensable for band-gap narrowing and photocatalytic activity, as assessed by first-principles calculations and x-ray photoemission spectroscopy.
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8 被引频次： 10558
题目：Electronics and optoelectronics of two-dimensional transition metal dichalcogenides
作者： Wang, QH (Wang, Qing Hua); Kalantar-Zadeh, K (Kalantar-Zadeh, Kourosh); Kis, A (Kis, Andras); Coleman, JN (Coleman, Jonathan N.); Strano, MS (Strano, Michael S.)
出处：NATURE NANOTECHNOLOGY
摘要：The remarkable properties of graphene have renewed interest in inorganic, two-dimensional

materials with unique electronic and optical attributes. Transition metal dichalcogenides (TMDCs) are layered materials with strong in-plane bonding and weak out-of-plane interactions enabling exfoliation into two-dimensional layers of single unit cell thickness. Although TMDCs have been studied for decades, recent advances in nanoscale materials characterization and device fabrication have opened up new opportunities for two-dimensional layers of thin TMDCs in nanoelectronics and optoelectronics. TMDCs such as MoS2, MoSe2, WS2 and WSe2 have sizable bandgaps that change from indirect to direct in single layers, allowing applications such as transistors, photodetectors and electroluminescent devices. We review the historical development of TMDCs, methods for preparing atomically thin layers, their electronic and optical properties, and prospects for future advances in electronics and optoelectronics.

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9　被引频次：　10277

题目：Single-layer MoS2 transistors

作者：Radisavljevic, B (Radisavljevic, B.); Radenovic, A (Radenovic, A.); Brivio, J (Brivio, J.); Giacometti, V (Giacometti, V.); Kis, A (Kis, A.)

出处：NATURE NANOTECHNOLOGY

摘要：Two-dimensional materials are attractive for use in next-generation nanoelectronic devices because, compared to one-dimensional materials, it is relatively easy to fabricate complex structures from them. The most widely studied two-dimensional material is graphene(1,2), both because of its rich physics(3-5) and its high mobility(6). However, pristine graphene does not have a bandgap, a property that is essential for many applications, including transistors(7). Engineering a graphene bandgap increases fabrication complexity and either reduces mobilities to the level of strained silicon films(8-13) or requires high voltages(14,15). Although single layers of MoS2 have a large intrinsic bandgap of 1.8 eV (ref. 16), previously reported mobilities in the 0.5-3 cm(2) V-1 s(-1) range(17) are too low for practical devices. Here, we use a halfnium oxide gate dielectric to demonstrate a room-temperature single-layer MoS2 mobility of at least 200 cm(2) V-1 s(-1), similar to that of graphene nanoribbons, and demonstrate transistors with room-temperature current on/off ratios of 1 x 10(8) and ultralow standby power dissipation. Because monolayer MoS2 has a direct bandgap(16,18), it can be used to construct interband tunnel FETs19, which offer lower power consumption than classical transistors. Monolayer MoS2 could also complement graphene in applications that require thin transparent semiconductors, such as optoelectronics and energy harvesting.

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10 被引频次： 8508
题目： Multiplex Genome Engineering Using CRISPR/Cas Systems
作者： Cong, L (Cong, Le); Ran, FA (Ran, F. Ann); Cox, D (Cox, David); Lin, SL (Lin, Shuailiang); Barretto, R (Barretto, Robert); Habib, N (Habib, Naomi); Hsu, PD (Hsu, Patrick D.); Wu, XB (Wu, Xuebing); Jiang, WY (Jiang, Wenyan); Marraffini, LA (Marraffini, Luciano A.); Zhang, F (Zhang, Feng)
出处： SCIENCE
摘要： Functional elucidation of causal genetic variants and elements requires precise genome editing technologies. The type II prokaryotic CRISPR (clustered regularly interspaced short palindromic repeats)/Cas adaptive immune system has been shown to facilitate RNA-guided site-specific DNA cleavage. We engineered two different type II CRISPR/Cas systems and demonstrate that Cas9 nucleases can be directed by short RNAs to induce precise cleavage at endogenous genomic loci in human and mouse cells. Cas9 can also be converted into a nicking enzyme to facilitate homology-directed repair with minimal mutagenic activity. Lastly, multiple guide sequences can be encoded into a single CRISPR array to enable simultaneous editing of several sites within the mammalian genome, demonstrating easy programmability and wide applicability of the RNA-guided nuclease technology.
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11 被引频次：8350
题目：The Chemistry and Applications of Metal-Organic Frameworks
作者： Furukawa, H (Furukawa, Hiroyasu); Cordova, KE (Cordova, Kyle E.); O'Keeffe, M (O'Keeffe, Michael); Yaghi, OM (Yaghi, Omar M.)
出处：SCIENCE
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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12 被引频次： 7328
题目：Graphene and Graphene Oxide: Synthesis, Properties, and Applications
作者：Zhu, YW (Zhu, Yanwu); Murali, S (Murali, Shanthi); Cai, WW (Cai, Weiwei); Li, XS (Li, Xuesong); Suk, JW (Suk, Ji Won); Potts, JR (Potts, Jeffrey R.); Ruoff, RS (Ruoff, Rodney S.)
出处：ADVANCED MATERIALS
摘要：There is intense interest in graphene in fields such as physics, chemistry, and materials science, among others. Interest in graphene's exceptional physical properties, chemical tunability, and potential for applications has generated thousands of publications and an accelerating pace of research, making review of such research timely. Here is an overview of the synthesis, properties, and applications of graphene and related materials (primarily, graphite oxide and its colloidal suspensions and materials made from them), from a materials science perspective.
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13 被引频次： 7212
题目： Sequential deposition as a route to high-performance perovskite-sensitized solar cell
作者： Burschka, J (Burschka, Julian); Pellet, N (Pellet, Norman); Moon, SJ (Moon, Soo-Jin); Humphry-Baker, R (Humphry-Baker, Robin); Gao, P (Gao, Peng); Nazeeruddin, MK (Nazeeruddin, Mohammad K.); Gratzel, M (Graetzel, Michael)
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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14 被引频次：6341

题目：The chemistry of two-dimensional layered transition metal dichalcogenide nanosheets

作者：Chhowalla, M (Chhowalla, Manish); Shin, HS (Shin, Hyeon Suk); Eda, G (Eda, Goki); Li, LJ (Li, Lain-Jong); Loh, KP (Loh, Kian Ping); Zhang, H (Zhang, Hua)

出处：NATURE CHEMISTRY

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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15 被引频次： 5331
题目：The Li-Ion Rechargeable Battery: A Perspective
作者：Goodenough, JB (Goodenough, John B.); Park, KS (Park, Kyu-Sung)
出处：JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
摘要： Each cell of a battery stores electrical energy as chemical energy in two electrodes, a reductant (anode) and an oxidant (cathode), separated by an electrolyte that transfers the ionic component of the chemical reaction inside the cell and forces the electronic component outside the battery. The output on discharge is an external electronic current I at a voltage V for a time Delta t. The chemical reaction of a rechargeable battery must be reversible on the application of a charging I and V. Critical parameters of a rechargeable battery are safety, density of energy that can be stored at a specific power input and retrieved at a specific power output, cycle and shelf life, storage efficiency, and cost of fabrication. Conventional ambient-temperature rechargeable batteries have solid electrodes and a liquid electrolyte. The positive electrode (cathode) consists of a host framework into which the mobile (working) cation is inserted reversibly over a finite solid solution range. The solid solution range, which is reduced at higher current by the rate of transfer of the working ion across electrode/electrolyte interfaces and within a host, limits the amount of charge per electrode formula unit that can be transferred over the time Delta t = Delta t(I). Moreover, the difference between energies of the LUMO and the HOMO of the electrolyte, i.e., electrolyte window, determines the maximum voltage for a long shelf and cycle life. The maximum stable voltage with an aqueous electrolyte is 1.5 V; the Li-ion rechargeable battery uses an organic electrolyte with a larger window, which increase the density of stored energy for a given Delta t. Anode or cathode electrochemical potentials outside the electrolyte window can increase V, but they require formation of a passivating surface layer that must be permeable to Li+ and capable of adapting rapidly to the changing electrode surface area as the electrode changes volume during cycling. A passivating surface layer adds to the impedance of the Li+ transfer across the electrode/electrolyte interface and lowers the cycle life of a battery cell. Moreover, formation of a passivation layer on the anode robs Li from the cathode irreversibly on an initial charge, further lowering the reversible Delta t. These problems plus the cost of quality control of manufacturing plague development of Li-ion rechargeable batteries that can compete with the internal combustion engine for powering electric cars and that can provide the needed low-cost storage of electrical energy generated by renewable wind and/or solar energy. Chemists are contributing to incremental improvements of the conventional strategy by investigating and controlling electrode passivation layers, improving the rate of Li+ transfer across electrode/electrolyte interfaces, identifying electrolytes with larger windows while retaining a Li+ conductivity sigma(Li) > 10(-3) S cm(-1), synthesizing electrode morphologies that reduce the size of the active particles while pinning them on current collectors of large surface area accessible by the electrolyte, lowering the cost of cell fabrication, designing displacement-reaction anodes of higher capacity that allow a safe, fast charge, and designing alternative cathode hosts. However, new strategies are needed for batteries that go beyond powering hand-held devices, such as using

electrode hosts with two-electron redox centers; replacing the cathode hosts by materials that undergo displacement reactions (e.g.
sulfur) by liquid cathodes that may contain flow-through redox molecules, or by catalysts for air cathodes; and developing a solid electrolyte separator membrane that allows an organic and aqueous liquid electrolyte on the anode and cathode sides, respectively. Opportunities exist for the chemist to bring together oxide and polymer or graphene chemistry in imaginative morphologies.
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16 被引频次：4963
题目：TiO2 photocatalysis and related surface phenomena
作者：Fujishima, A (Fujishima, Akira); Zhang, XT (Zhang, Xintong); Tryk, DA (Tryk, Donald A.)
出处：SURFACE SCIENCE REPORTS
摘要：The field of photocatalysis can be traced back more than 80 years to early observations of the chalking of titania-based paints and to studies of the darkening of metal oxides in contact with organic compounds in sunlight. During the past 20 years, it has become an extremely well researched field due to practical interest in air and water remediation, self-cleaning surfaces, and self-sterilizing surfaces. During the same period, there has also been a strong effort to use photocatalysis for light-assisted production of hydrogen. The fundamental aspects of photocatalysis on the most studied photocatalyst, titania, are still being actively researched and have recently become quite well understood. The mechanisms by which certain types of organic compounds are decomposed completely to carbon dioxide and water, for example, have been delineated. However, certain aspects, such as the photo-induced wetting phenomenon, remain controversial, with some groups maintaining that the effect is a simple one in which organic contaminants are decomposed, while other groups maintain that there are additional effects in which the intrinsic surface properties are modified by light. During the past several years, powerful tools such as surface spectroscopic techniques and scanning probe techniques performed on single crystals in ultra-high vacuum, and ultrafast pulsed laser spectroscopic techniques have been brought to bear on these problems, and new insights have become possible. Quantum chemical calculations have also provided new insights. New materials have recently been developed based on titania, and the sensitivity to visible light has improved. The new information available is staggering, but we hope to Offer an overview of some of the recent highlights, as well as to review some of the origins and indicate some possible new directions. (C) 2008 Elsevier B.V. All rights reserved
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17 被引频次：4380

题目：Co3O4 nanocrystals on graphene as a synergistic catalyst for oxygen reduction reaction

作者：Liang, YY (Liang, Yongye); Li, YG (Li, Yanguang); Wang, HL (Wang, Hailiang); Zhou, JG (Zhou, Jigang); Wang, J (Wang, Jian); Regier, T (Regier, Tom); Dai, HJ (Dai, Hongjie)

出处：NATURE MATERIALS

摘要： Catalysts for oxygen reduction and evolution reactions are at the heart of key renewable-energy technologies including fuel cells and water splitting. Despite tremendous efforts, developing oxygen electrode catalysts with high activity at low cost remains a great challenge. Here, we report a hybrid material consisting of Co3O4 nanocrystals grown on reduced graphene oxide as a high-performance bi-functional catalyst for the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER). Although Co3O4 or graphene oxide alone has little catalytic activity, their hybrid exhibits an unexpected, surprisingly high ORR activity that is further enhanced by nitrogen doping of graphene. The Co3O4/N-doped graphene hybrid exhibits similar catalytic activity but superior stability to Pt in alkaline solutions. The same hybrid is also highly active for OER, making it a high-performance non-precious metal-based bi-catalyst for both ORR and OER. The unusual catalytic activity arises from synergetic chemical coupling effects between Co3O4 and graphene.

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18 被引频次：3606

题目：Advanced Materials for Energy Storage

作者： Liu, C (Liu, Chang); Li, F (Li, Feng); Ma, LP (Ma, Lai-Peng); Cheng, HM (Cheng, Hui-Ming)

摘要： Popularization of portable electronics and electric vehicles worldwide stimulates the development of energy storage devices, such as batteries and supercapacitors, toward higher power density and energy density, which significantly depends upon the advancement of new materials used in these devices. Moreover, energy storage materials play a key role in efficient, clean, and versatile use of energy, and are crucial for the exploitation of renewable energy. Therefore, energy storage materials cover a wide range of materials and have been receiving intensive attention from research and development to industrialization. In this Review, firstly a general introduction is given to several typical energy storage systems, including thermal, mechanical, electromagnetic, hydrogen, and electrochemical energy storage. Then the current status of high-performance hydrogen storage materials for on-board applications and electrochemical energy storage materials for lithium-ion batteries and supercapacitors is introduced in detail. The strategies for developing these advanced energy storage materials, including nanostructuring nano-/microcombination, hybridization, pore-structure control, configuration design, surface modification, and composition optimization, are discussed. Finally, the future trends and prospects in the development of advanced energy storage materials are highlighted.

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19 被引频次：3492
题目：Coral reefs under rapid climate change and ocean acidification
作者：Hoegh-Guldberg, O (Hoegh-Guldberg, O.); Mumby, PJ (Mumby, P. J.); Hooten, AJ (Hooten, A. J.); Steneck, RS (Steneck, R. S.); Greenfield, P (Greenfield, P.); Gomez, E (Gomez, E.); Harvell, CD (Harvell, C. D.); Sale, PF (Sale, P. F.); Edwards, AJ (Edwards, A. J.); Caldeira, K (Caldeira, K.); Knowlton, N (Knowlton, N.); Eakin, CM (Eakin, C. M.); Iglesias-Prieto, R (Iglesias-Prieto, R.); Muthiga, N (Muthiga, N.); Bradbury, RH (Bradbury, R. H.); Dubi, A (Dubi, A.); Hatziolos, ME (Hatziolos, M. E.)
出处：SCIENCE
摘要：Atmospheric carbon dioxide concentration is expected to exceed 500 parts per million and global temperatures to rise by at least 2 degrees C by 2050 to 2100, values that significantly exceed those of at least the past 420,000 years during which most extant marine organisms evolved. Under conditions expected in the 21st century, global warming and ocean acidification will compromise carbonate accretion, with corals becoming increasingly rare on reef systems. The result will be less diverse reef communities and carbonate reef structures that fail to be maintained. Climate change also exacerbates local stresses from declining water quality and overexploitation of key species, driving reefs increasingly toward the tipping point for functional collapse. This review presents future scenarios for coral reefs that predict increasingly serious consequences for reef- associated fisheries, tourism, coastal protection, and people. As the International Year of the Reef 2008 begins, scaled- up management intervention and decisive action on global emissions are required if the loss of coral- dominated ecosystems is to be avoided.
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20 被引频次： 3480

题目：Graphitic Carbon Nitride (g-C3N4)-Based Photocatalysts for Artificial Photosynthesis and Environmental Remediation: Are We a Step Closer To Achieving Sustainability?

作者：Ong, WJ (Ong, Wee-Jun); Tan, LL (Tan, Lling-Lling); Ng, YH (Ng, Yun Hau); Yong, ST (Yong, Siek-Ting); Chai, SP (Chai, Siang-Piao)

出处：CHEMICAL REVIEWS

摘要：As a fascinating conjugated polymer, graphitic carbon nitride (g-C3N4) has become a new research hotspot and drawn broad interdisciplinary attention as a metal-free and visible-light-responsive photocatalyst in the arena of solar energy conversion and environmental remediation. This is due to its appealing electronic band structure, high physicochemical stability, and "earth-abundant" nature. This critical review summarizes a panorama of the latest progress related to the design and construction of pristine g-C3N4 and g-C3N4-based nanocomposites, including (1) nanoarchitecture design of bare g-C3N4, such as hard and soft templating approaches, supramolecular preorganization assembly, exfoliation, and template-free synthesis routes, (2) functionalization of g-C3N4 at an atomic level (elemental doping) and molecular level (copolymerization), and (3) modification of g-C3N4 with well-matched energy levels of another semiconductor or a metal as a cocatalyst to form heterojunction nanostructures. The construction and characteristics of each classification of the heterojunction system will be critically reviewed, namely metal-g-C3N4, semiconductor-g-C3N4, isotype g-C3N4/g-C3N4, graphitic carbon-g-C3N4, conducting polymer-g-C3N4, sensitizer-g-C3N4, and multicomponent heterojunctions. The band structures, electronic properties, optical absorption, and interfacial charge transfer of g-C3N4-based heterostructured nanohybrids will also be theoretically discussed based on the first-principles density functional theory (DFT) calculations to provide insightful outlooks on the charge carrier dynamics. Apart from that, the advancement of the versatile photoredox applications toward artificial photosynthesis (water splitting and photofixation of CO2), environmental decontamination, and bacteria disinfection will be presented in detail. Last but not least, this comprehensive review will conclude with a summary and some invigorating perspectives on the challenges and future directions at the forefront of this research platform. It is anticipated that this review can stimulate a new research doorway to facilitate the next generation of gC(3)N(4)-based photocatalysts with ameliorated performances by harnessing the outstanding structural, electronic, and optical properties for the development of a sustainable future without environmental detriment.

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21 被引频次：3426

题目：Noble metal-free hydrogen evolution catalysts for water splitting

作者：Zou, XX (Zou, Xiaoxin); Zhang, Y (Zhang, Yu)

出处：CHEMICAL SOCIETY REVIEWS

摘要：Sustainable hydrogen production is an essential prerequisite of a future hydrogen economy. Water electrolysis driven by renewable resource-derived electricity and direct solar-to-hydrogen conversion based on photochemical and photoelectrochemical water splitting are promising pathways for sustainable hydrogen production. All these techniques require, among many things, highly active noble metal-free hydrogen evolution catalysts to make the water splitting process more energy-efficient and economical. In this review, we highlight the recent research efforts toward the synthesis of noble metal-free electrocatalysts, especially at the nanoscale, and their catalytic properties for the hydrogen evolution reaction (HER). We review several important kinds of heterogeneous non-precious metal electrocatalysts, including metal sulfides, metal selenides, metal carbides, metal nitrides, metal phosphides, and heteroatom-doped nanocarbons. In the discussion, emphasis is given to the synthetic methods of these HER electrocatalysts, the strategies of performance improvement, and the structure/composition-catalytic activity relationship. We also summarize some important examples showing that non-Pt HER electrocatalysts could serve as efficient cocatalysts for promoting direct solar-to-hydrogen conversion in both photochemical and photoelectrochemical water splitting systems, when combined with suitable semiconductor photocatalysts.

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22 被引频次： 3295

题目：Progress, Challenges, and Opportunities in Two-Dimensional Materials Beyond Graphene

作者：Butler, SZ (Butler, Sheneve Z.); Hollen, SM (Hollen, Shawna M.); Cao, LY (Cao, Linyou); Cui, Y (Cui, Yi); Gupta, JA (Gupta, Jay A.); Gutierrez, HR (Gutierrez, Humberto R.); Heinz, TF (Heinz, Tony F.); Hong, SS (Hong, Seung Sae); Huang, JX (Huang, Jiaxing); Ismach, AF (Ismach, Ariel F.); Johnston-Halperin, E (Johnston-Halperin, Ezekiel); Kuno, M (Kuno, Masaru); Plashnitsa, VV (Plashnitsa, Vladimir V.); Robinson, RD (Robinson, Richard D.); Ruoff, RS (Ruoff, Rodney S.); Salahuddin, S (Salahuddin, Sayeef); Shan, J (Shan, Jie); Shi, L (Shi, Li); Spencer, MG (Spencer, Michael G.); Terrones, M (Terrones, Mauricio); Windl, W (Windl, Wolfgang); Goldberger, JE (Goldberger, Joshua E.)

出处：ACS NANO

摘要：Graphene's success has shown that it is possible to create stable, single and few-atom-thick layers of van der Waals materials, and also that these materials can exhibit fascinating and technologically useful properties. Here we review the state-of-the-art of 2D materials beyond

graphene. Initially, we will outline the different chemical classes of 2D materials and discuss the various strategies to prepare single-layer, few-layer, and multilayer assembly materials in solution, on substrates, and on the wafer scale. Additionally, we present an experimental guide for identifying and characterizing single-layer-thick materials, as well as outlining emerging techniques that yield both local and global information. We describe the differences that occur in the electronic structure between the bulk and the single layer and discuss various methods of tuning their electronic properties by manipulating the surface. Finally, we highlight the properties and advantages of single-, few-, and many-layer 2D materials in field-effect transistors, spin- and valley-tronics, thermoelectrics, and topological insulators, among many other applications.

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23 被引频次： 2624

题目：Recent Advances in Ultrathin Two-Dimensional Nanomaterials

作者：Tan, CL (Tan, Chaoliang); Cao, XH (Cao, Xiehong); Wu, XJ (Wu, Xue-Jun); He, QY (He, Qiyuan); Yang, J (Yang, Jian); Zhang, X (Zhang, Xiao); Chen, JZ (Chen, Junze); Zhao, W (Zhao, Wei); Han, SK (Han, Shikui); Nam, GH (Nam, Gwang-Hyeon); Sindoro, M (Sindoro, Melinda); Zhang, H (Zhang, Hua)

出处：CHEMICAL REVIEWS

摘要：Since the discovery of mechanically exfoliated graphene in 2004, research on ultrathin two-dimensional (2D) nanomaterials has grown exponentially in the fields of condensed matter physics, material science, chemistry, and nanotechnology. Highlighting their compelling physical,

chemical, electronic, and optical properties, as well as their various potential applications, in this Review, we summarize the state-of-art progress on the ultrathin 2D nanomaterials with a particular emphasis on their recent advances. First, we introduce the unique advances on ultrathin 2D nanomaterials, followed by the description of their composition and crystal structures. The assortments of their synthetic methods are then summarized, including insights on their advantages and limitations, alongside some recommendations on suitable characterization techniques. We also discuss in detail the utilization of these ultrathin 2D nanomaterials for wide ranges of potential applications among the electronics/optoelectronics, electrocatalysis, batteries, supercapacitors, solar cells, photo catalysis, and sensing platforms. Finally, the challenges and outlooks in this promising field are featured on the basis of its current development.

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24 被引频次：1118

题目：ON THE DEPLETION OF ANTARCTIC OZONE

作 者： SOLOMON, S (SOLOMON, S); GARCIA, RR (GARCIA, RR); ROWLAND, FS (ROWLAND, FS); WUEBBLES, DJ (WUEBBLES, DJ)

出处：NATURE

摘要：Recent observations by Farman et al.1 reveal remarkable depletions in the total atmospheric ozone content in Antarctica. The observed total ozone decreased smoothly during the period from about 1975 to the present, but only in the spring season. The observed ozone content at Halley Bay was ～30% lower in the Antarctic spring seasons (October) of 1980–84 than in the springs of 1957–73. No such obvious perturbation is observable in other seasons, or at other than the very highest latitudes in the Southern Hemisphere, and the magnitude of the observed change there far exceeds climatological variability2. We present here balloonsonde ozone data3,4 which show that these ozone changes are largely confined to the region from about 10 to 20 km, during the period August to October. We show that homogeneous (gas phase) chemistry as presently understood cannot explain these observed depletions. On the other hand, a unique feature of the Antarctic lower stratosphere is its high frequency of polar stratospheric clouds5, providing a reaction site for heterogeneous reactions. A heterogeneous reaction between HCl and ClONO2 is explored as a possible mechanism to explain the ozone observations. This process produces changes in ozone that are consistent with the observations, and its implications for the behaviour of HNO3 and NO2 in the Antarctic stratosphere are consistent with observations of those species there, providing an important check on the proposed mechanism. Similar ozone changes are obtained with another possible heterogeneous reaction, H2O + ClONO2.

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25 被引频次：18

题目：A sparse and high-order accurate line-based discontinuous Galerkin method for unstructured meshes

作者：Persson, PO (Persson, Per-Olof)

出处：JOURNAL OF COMPUTATIONAL PHYSICS

摘要： We present a new line-based discontinuous Galerkin (DG) discretization scheme for first- and second-order systems of partial differential equations. The scheme is based on fully unstructured meshes of quadrilateral or hexahedral elements, and it is closely related to the standard nodal DG scheme as well as several of its variants such as the collocation- based DG spectral element method (DGSEM) or the spectral difference (SD) method. However, our motivation is to maximize the sparsity of the Jacobian matrices, since this directly translates into higher performance in particular for implicit solvers, while maintaining many of the good properties of the DG scheme. To achieve this, our scheme is based on applying one-dimensional DG solvers along each coordinate direction in a reference element. This reduces the number of connectivities drastically, since the scheme only connects each node to a line of nodes along each direction, as opposed to the standard DG method which connects all nodes inside the element and many nodes in the neighboring ones. The resulting scheme is similar to a collocation scheme, but it uses fully consistent integration along each 1-D coordinate direction which results in different properties for nonlinear problems and curved elements. Also, the scheme uses solution points along each element face, which further reduces the number of connections with the neighboring elements. Second-order terms are handled by an LDG-type approach, with an upwind/downwind flux function based on a switch function at each element face. We demonstrate the accuracy of the method and compare it to the standard nodal DG method for problems including Poisson's equation, Euler's equations of gas dynamics, and both the steady-state and the transient compressible Navier-Stokes equations. We also show how to integrate the Navier-Stokes equations using implicit schemes and Newton-Krylov solvers, without impairing the high sparsity of the matrices.

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ESI HIGHLY CITED PAPERS

(Chemistry)

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

1 被引频次： 77505
题目： A short history of SHELX
作者： Sheldrick, GM (Sheldrick, George M.)
出处： ACTA CRYSTALLOGRAPHICA A-FOUNDATION AND ADVANCES
摘要： An account is given of the development of the SHELX system of computer programs from SHELX-76 to the present day. In addition to identifying useful innovations that have come into general use through their implementation in SHELX, a critical analysis is presented of the less-successful features, missed opportunities and desirable improvements for future releases of the software. An attempt is made to understand how a program originally designed for photographic intensity data, punched cards and computers over 10000 times slower than an average modern personal computer has managed to survive for so long. SHELXL is the most widely used program for small-molecule refinement and SHELXS and SHELXD are often employed for structure solution despite the availability of objectively superior programs. SHELXL also finds a niche for the refinement of macromolecules against high-resolution or twinned data; SHELXPRO acts as an interface for macromolecular applications. SHELXC, SHELXD and SHELXE are proving useful for the experimental phasing of macromolecules, especially because they are fast and robust and so are often employed in pipelines for high-throughput phasing. This paper could serve as a general literature citation when one or more of the open-source SHELX programs (and the Bruker AXS version SHELXTL) are employed in the course of a crystal-structure determination.
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2 被引频次： 54962
题目： Gapped BLAST and PSI-BLAST: a new generation of protein database search programs
作者： Altschul, SF (Altschul, SF); Madden, TL (Madden, TL); Schaffer, AA (Schaffer, AA); Zhang, JH (Zhang, JH); Zhang, Z (Zhang, Z); Miller, W (Miller, W); Lipman, DJ (Lipman, DJ)
出处： NUCLEIC ACIDS RESEARCH
摘要： The BLAST programs are widely used tools for searching protein and DNA databases for sequence similarities. For protein comparisons, a variety of definitional, algorithmic and statistical refinements described here permits the execution time of the BLAST programs to be

decreased substantially while enhancing their sensitivity to weak similarities, A new criterion for triggering the extension of word hits, combined with a new heuristic for generating gapped alignments, yields a gapped BLAST program that runs at approximately three times the speed of the original, In addition, a method is introduced for automatically combining statistically significant alignments produced by BLAST into a position-specific score matrix, and searching the database using this matrix, The resulting Position-Specific Iterated BLAST (PSI-BLAST) program runs at approximately the same speed per iteration as gapped BLAST, but in many cases is much more sensitive to weak but biologically relevant sequence similarities. PSI-BLAST is used to uncover several new and interesting members of the BRCT superfamily.

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3 被引频次： 52651

题目： CLUSTAL-W - IMPROVING THE SENSITIVITY OF PROGRESSIVE MULTIPLE SEQUENCE ALIGNMENT THROUGH SEQUENCE WEIGHTING, POSITION-SPECIFIC GAP PENALTIES AND WEIGHT MATRIX CHOICE

作者： THOMPSON, JD (THOMPSON, JD); HIGGINS, DG (HIGGINS, DG); GIBSON, TJ (GIBSON, TJ)

出处： NUCLEIC ACIDS RESEARCH

摘要： The sensitivity of the commonly used progressive multiple sequence alignment method has been greatly improved for the alignment of divergent protein sequences, Firstly, individual weights are assigned to each sequence in a partial alignment in order to down-weight near-duplicate sequences and up-weight the most divergent ones. Secondly, amino acid substitution matrices are varied at different alignment stages according to the divergence of the sequences to be aligned. Thirdly, residue-specific gap penalties and locally reduced gap penalties in hydrophilic regions encourage new gaps in potential loop regions rather than regular secondary structure. Fourthly, positions in early alignments where gaps have been opened receive locally reduced gap penalties to encourage the opening up of new gap at these positions. These modifications are incorporated into a new program, CLUSTAL W which is freely available.

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4 被引频次： 37082

题目： STATISTICAL METHODS FOR ASSESSING AGREEMENT BETWEEN TWO METHODS OF CLINICAL MEASUREMENT

作者： BLAND, JM (BLAND, JM); ALTMAN, DG (ALTMAN, DG)

出处： LANCET

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摘要：In clinical measurement comparison of a new measurement technique with an established one is often needed to see whether they agree sufficiently for the new to replace the old. Such investigations are often analysed inappropriately, notably by using correlation coefficients. The

use of correlation is misleading. An alternative approach, based on graphical techniques and simple calculations, is described, together with the relation between this analysis and the assessment of repeatability.

5 被引频次： 33048
题目： VMD: Visual molecular dynamics
作者： Humphrey, W (Humphrey, W); Dalke, A (Dalke, A); Schulten, K (Schulten, K)
出处： JOURNAL OF MOLECULAR GRAPHICS & MODELLING
摘要： VMD is a molecular graphics program designed for the display and analysis of molecular assemblies, in particular biopolymers such as proteins and nucleic acids. VMD can simultaneously display any number of structures using a wide variety of rendering styles and coloring methods. Molecules are displayed as one or more "representations," in which each representation embodies a particular rendering method and coloring scheme for a selected subset of atoms. The atoms displayed in each representation are chosen using an extensive atom selection syntax, which includes Boolean operators and regular expressions. VMD provides a complete graphical user interface for program control, as well as a text interface using the Tcl embeddable parser to allow for complex scripts with variable substitution, control loops, and function calls. Full session logging is supported, which produces a VMD command script for later playback. High-resolution raster images of displayed molecules may be produced by generating input scripts for use by a number of photorealistic image-rendering applications. VMD has also been expressly designed with the ability to animate molecular dynamics (MD) simulation trajectories, imported either from files or from a direct connection to a running MD simulation. VMD is the visualization component of MDScope, a set of tools for interactive problem solving in structural biology, which also includes the parallel MD program NAMD, and the MDCOMM software used to connect the visualization and simulation programs. VMD is written in C++, using an object-oriented design; the program, including source code and extensive documentation, is freely available via anonymous ftp and through the World Wide Web.
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6 被引频次： 26321
题目：FAST PARALLEL ALGORITHMS FOR SHORT-RANGE MOLECULAR-DYNAMICS
作者： PLIMPTON, S (PLIMPTON, S)
出处： JOURNAL OF COMPUTATIONAL PHYSICS
摘要： Three parallel algorithms for classical molecular dynamics are presented. The first assigns each processor a fixed subset of atoms; the second assigns each a fixed subset of inter-atomic forces to compute; the third assigns each a fixed spatial region, The algorithms are suitable for molecular dynamics models which can be difficult to parallelize efficiently-those with short-range forces where the neighbors of each atom change rapidly, They can be implemented on any distributed-memory parallel machine which allows for message-passing of data between independently executing processors. The algorithms are tested on a standard Lennard-Jones benchmark problem for system sizes ranging from 500 to 100,000,000 atoms on several parallel supercomputers-the nCUBE 2, Intel iPSC/860 and Paragon, and Cray T3D. Comparing the results

to the fastest reported vectorized Gray Y-MP and C90 algorithm shows that the current generation of parallel machines is competitive with conventional vector supercomputers even for small problems, for large problems, the spatial algorithm achieves parallel efficiencies of 90% and a 1840-node Intel Paragon performs up to 165 faster than a single Gray C90 processor. Trade-offs between the three algorithms and guidelines for adapting them to more complex molecular dynamics simulations are also discussed. (C) 1995 Academic Press, Inc.

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7 被引频次： 24324

题目： The Protein Data Bank

作者： Berman, HM (Berman, HM); Westbrook, J (Westbrook, J); Feng, Z (Feng, Z); Gilliland, G (Gilliland, G); Bhat, TN (Bhat, TN); Weissig, H (Weissig, H); Shindyalov, IN (Shindyalov, IN); Bourne, PE (Bourne, PE)

出处： NUCLEIC ACIDS RESEARCH

摘要： The Protein Data Bank (PDB; http://www.rcsb.org/pdb/) is the-single worldwide archive of structural data of biological macromolecules. This paper describes the goals of the PDB, the systems in place for data deposition and access, how to obtain further information, and near-term plans for the future development of the resource.

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8 被引频次： 23898

题目： RELIABILITY OF MOLECULAR WEIGHT DETERMINATIONS BY DODECYL SULFATE-POLYACRYLAMIDE GEL ELECTROPHORESIS

作者： WEBER, K (WEBER, K); OSBORN, M (OSBORN, M)

出处： JOURNAL OF BIOLOGICAL CHEMISTRY

摘要： Forty proteins with polypeptide chains of well characterized molecular weights have been studied by polyacrylamide gel electrophoresis in the presence of sodium dodecyl sulfate following the procedure of Shapiro, Viñuela, and Maizel (Biochem. Biophys. Res. Commun., 28, 815 (1967)). When the electrophoretic mobilities were plotted against the logarithm of the known polypeptide chain molecular weights, a smooth curve was obtained. The results show that the method can be used with great confidence to determine the molecular weights of polypeptide chains for a wide variety of proteins.

9 被引频次： 23487
题目： ELECTROCHEMICAL PHOTOLYSIS OF WATER AT A SEMICONDUCTOR ELECTRODE
作者： FUJISHIMA, A (FUJISHIMA, A); HONDA, K (HONDA, K)
出处： NATUR
摘要： ALTHOUGH the possibility of water photolysis has been investigated by many workers, a useful method has only now been developed. Because water is transparent to visible light it cannot be decomposed directly, but only by radiation with wavelengths shorter than 190 nm (ref. 1).

10 被引频次： 22950
题目： ESTIMATION OF CONCENTRATION OF LOW-DENSITY LIPOPROTEIN CHOLESTEROL IN PLASMA, WITHOUT USE OF PREPARATIVE ULTRACENTRIFUGE
作者： FRIEDEWALD, WT (FRIEDEWALD, WT); FREDRICKSON, DS (FREDRICKSON, DS); LEVY, RI (LEVY, RI)
出处： CLINICAL CHEMISTRY
摘要： A method for estimating the cholesterol content of the serum low-density lipoprotein fraction (Sf0-20) is presented. The method involves measurements of fasting plasma total cholesterol, triglyceride, and high-density lipoprotein cholesterol concentrations, none of which requires the use of the preparative ultracentrifuge. Comparison of this suggested procedure with the more direct procedure, in which the ultracentrifuge is used, yielded correlation coefficients of .94 to .99, depending on the patient population compared.

11 被引频次： 21812
题目： TISSUE SULFHYDRYL GROUPS
作者： ELLMAN, GL (ELLMAN, GL)
出处： CLINICAL CHEMISTRY
摘要： A water-soluble (at pH 8) aromatic disulfide [5,5′ -dithiobis(2-nitrobenzoic acid)] has been synthesized and shown to be useful for determination of sulfhydryl groups. Several applications have been made to show its usefulness for biological materials. A study of the reaction of this disulfide with blood has produced some evidence for the splitting of disulfide bonds by reduced heme.

12 被引频次： 20944
题目： A NEW AND RAPID COLORIMETRIC DETERMINATION OF ACETYLCHOLINESTERASE ACTIVITY
作者： ELLMAN, GL (ELLMAN, GL); COURTNEY, KD (COURTNEY, KD); ANDRES, V (ANDRES, V); FEATHERSTONE, RM (FEATHERSTONE, RM)
出处： BIOCHEMICAL PHARMACOLOGY
摘要： A photometric method for determining acetylcholinesterase activity of tissue extracts, homogenates, cell suspensions, etc., has been described. The enzyme activity is measured by following the increase of yellow color produced from thiocholine when it reacts with dithiobisnitrobenzoate ion. It is based on coupling of these reactions:The latter reaction is rapid

and the assay is sensitive (i.e. a 10 μ 1 sample of blood is adequate). The use of a recorder has been most helpful, but is not essential. The method has been used to study the enzyme in human erythrocytes and homogenates of rat brain, kidney, lungs, liver and muscle tissue. Kinetic constants determined by this system for erythrocyte eholinesterase are presented. The data obtained with acetylthiocholine as substrate are similar to those with acetylcholine.

13 被引频次： 20290

题目： Cytoscape: A software environment for integrated models of biomolecular interaction networks

作者： Shannon, P (Shannon, P); Markiel, A (Markiel, A); Ozier, O (Ozier, O); Baliga, NS (Baliga, NS); Wang, JT (Wang, JT); Ramage, D (Ramage, D); Amin, N (Amin, N); Schwikowski, B (Schwikowski, B); Ideker, T (Ideker, T)

出处： GENOME RESEARCH

摘要： Cytoscape is an open source software project for integrating biomolecular interaction networks with high-throughput expression data and other Molecular states into a unified conceptual framework. Although applicable to any system of molecular components and interactions, Cytoscape is most powerful when used in Conjunction with large databases of protein-protein, protein-DNA, and genetic interactions that are increasingly available for humans and model organisms. Cytoscape's software Core provides basic functionality to layout and query the network; to Visually integrate the network with expression profiles, phenotypes, and other molecular states; and to link the network to databases of functional annotations. The Core is extensible through a straightforward plug-in architecture, allowing rapid development of additional Computational analyses and features. Several case Studies of Cytoscape plug-ins are Surveyed, including a search for interaction pathways correlating with changes in gene expression, a Study of protein complexes involved in cellular recovery to DNA damage, inference of a combined physical/functional interaction network for Halobacterium, and an interface to detailed stochastic/kinetic gene regulatory models.

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14 被引频次： 19760

题目： PHASE ANNEALING IN SHELX-90 - DIRECT METHODS FOR LARGER STRUCTURES

作者： SHELDRICK, GM (SHELDRICK, GM)

出处： ACTA CRYSTALLOGRAPHICA SECTION A

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摘要： A number of extensions to the multisolution approach to the crystallographic phase problem are discussed in which the negative quartet relations play an important role. A phase annealing method, related to the simulated annealing approach in other optimization problems, is proposed and it is shown that it can result in an improvement of up to an order of magnitude in the

chances of solving large structures at atomic resolution. The ideas presented here are incorporated in the program system SHELX-90; the philosophical and mathematical background to the direct-methods part (SHELXS) of this system is described

15 被引频次：18374

题目： Semiempirical GGA-type density functional constructed with a long-range dispersion correction

作者： Grimme, S (Grimme, Stefan)

出处： JOURNAL OF COMPUTATIONAL CHEMISTRY

摘要： A new density functional (DF) of the generalized gradient approximation (GGA) type for general chemistry applications termed B97-D is proposed. It is based on Becke's power-series ansatz from 1997 and is explicitly parameterized by including damped atom-pairwise dispersion corrections of the form C-6 . R-6. A general computational scheme for the parameters used in this correction has been established and parameters for elements up to xenon and a scaling factor for the dispersion part for several common density functionals (BLYP, PBE, TPSS, B3LYP) are reported. The new functional is tested in comparison with other GGAs and the B3LYP hybrid functional on standard thermochemical benchmark sets, for 40 noncovalently bound complexes, including large stacked aromatic molecules and group 11 element clusters, and for the computation of molecular geometries. Further cross-validation tests were performed for organometallic reactions and other difficult problems for standard functionals. In summary, it is found that B97-D belongs to one of the most accurate general purpose GGAs, reaching, for example for the G97/2 set of heat of formations, a mean absolute deviation of only 3.8 kcal mol(-1). The performance for noncovalently bound systems including many pure van der Waals complexes is exceptionally good, reaching on the average CCSD(T) accuracy. The basic strategy in the development to restrict the density functional description to shorter electron correlation lengths scales and to describe situations with medium to large interatomic distances by damped C-6 . R-6 terms seems to be very successful, as demonstrated for some notoriously difficult reactions. As an example, for the isomerization of larger branched to linear alkanes, B97-D is the only DF available that yields the right sign for the energy difference. From a practical point of view, the new functional seems to be quite robust and it is thus suggested as an efficient and accurate quantum chemical method for large systems where dispersion forces are of general importance. (C) 2006 Wiley Periodicals, Inc.

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16 被引频次： 18285

题目： The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals

作者： Zhao, Y (Zhao, Yan); Truhlar, DG (Truhlar, Donald G.)

出处： THEORETICAL CHEMISTRY ACCOUNTS

摘要： We present two new hybrid meta exchange-correlation functionals, called M06 and M06-2X. The M06 functional is parametrized including both transition metals and nonmetals,

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

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17 被引频次： 18225
题目： GENERAL ATOMIC AND MOLECULAR ELECTRONIC-STRUCTURE SYSTEM
作者： SCHMIDT, MW (SCHMIDT, MW); BALDRIDGE, KK (BALDRIDGE, KK); BOATZ, JA (BOATZ, JA); ELBERT, ST (ELBERT, ST); GORDON, MS (GORDON, MS); JENSEN, JH (JENSEN, JH); KOSEKI, S (KOSEKI, S); MATSUNAGA, N (MATSUNAGA, N); NGUYEN, KA (NGUYEN, KA); SU, SJ (SU, SJ); WINDUS, TL (WINDUS, TL); DUPUIS, M (DUPUIS, M); MONTGOMERY, JA (MONTGOMERY, JA)
出处： JOURNAL OF COMPUTATIONAL CHEMISTRY
摘要： A description of the ab initio quantum chemistry package GAMESS is presented. Chemical systems containing atoms through radon can be treated with wave functions ranging from the simplest closed-shell case up to a general MCSCF case, permitting calculations at the necessary level of sophistication. Emphasis is given to novel features of the program. The parallelization strategy used in the RHF, ROHF, UHF, and GVB sections of the program is described, and detailed speedup results are given. Parallel calculations can be run on ordinary workstations as well as dedicated parallel machines. (C) 1993 by John Wiley & Sons, Inc.
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18 被引频次： 17765
题目： DETERMINATION OF SERUM PROTEINS BY MEANS OF THE BIURET REACTION
作者： GORNALL, AG (GORNALL, AG); BARDAWILL, CJ (BARDAWILL, CJ); DAVID, MM (DAVID, MM)
出处： JOURNAL OF BIOLOGICAL CHEMISTRY

19 被引频次： 16857
题目： Clinical features of patients infected with 2019 novel coronavirus in Wuhan, China
作者： Huang, CL (Huang, Chaolin); Wang, YM (Wang, Yeming); Li, XW (Li, Xingwang); Ren, LL (Ren, Lili); Zhao, JP (Zhao, Jianping); Hu, Y (Hu, Yi); Zhang, L (Zhang, Li); Fan, GH (Fan, Guohui); Xu, JY (Xu, Jiuyang); Gu, XY (Gu, Xiaoying); Cheng, ZS (Cheng, Zhenshun); Yu, T (Yu, Ting); Xia, JA (Xia, Jiaan); Wei, Y (Wei, Yuan); Wu, WJ (Wu, Wenjuan); Xie, XL (Xie, Xuelei); Yin, W (Yin, Wen); Li, H (Li, Hui); Liu, M (Liu, Min); Xiao, Y (Xiao, Yan); Gao, H (Gao, Hong); Guo, L (Guo, Li); Xie, JG (Xie, Jungang); Wang, GF (Wang, Guangfa); Jiang, RM (Jiang, Rongmeng); Gao, ZC (Gao, Zhancheng); Jin, Q (Jin, Qi); Wang, JW (Wang, Jianwei); Cao, B (Cao, Bin)
出处： LANCET
摘要： Background A recent cluster of pneumonia cases in Wuhan, China, was caused by a novel betacoronavirus, the 2019 novel coronavirus (2019-nCoV). We report the epidemiological, clinical, laboratory, and radiological characteristics and treatment and clinical outcomes of these patients.
Methods All patients with suspected 2019-nCoV were admitted to a designated hospital in Wuhan. We prospectively collected and analysed data on patients with laboratory-confirmed 2019-nCoV infection by real-time RT-PCR and next-generation sequencing. Data were obtained with standardised data collection forms shared by WHO and the International Severe Acute Respiratory and Emerging Infection Consortium from electronic medical records. Researchers also directly communicated with patients or their families to ascertain epidemiological and symptom data. Outcomes were also compared between patients who had been admitted to the intensive care unit (ICU) and those who had not.
Findings By Jan 2, 2020, 41 admitted hospital patients had been identified as having laboratory-confirmed 2019-nCoV infection. Most of the infected patients were men (30 [73%] of 41); less than half had underlying diseases (13 [32%]), including diabetes (eight [20%]), hypertension (six [15%]), and cardiovascular disease (six [15%]). Median age was 49.0 years (IQR 41.0-58.0). 27 (66%) of 41 patients had been exposed to Huanan seafood market. One family cluster was found. Common symptoms at onset of illness were fever (40 [98%] of 41 patients), cough (31 [76%]), and myalgia or fatigue (18 [44%]); less common symptoms were sputum production (11 [28%] of 39), headache (three [8%] of 38), haemoptysis (two [5%] of 39), and diarrhoea (one [3%] of 38). Dyspnoea developed in 22 (55%) of 40 patients (median time from illness onset to dyspnoea 8.0 days [IQR 5.0-13.0]). 26 (63%) of 41 patients had lymphopenia. All 41 patients had pneumonia with abnormal findings on chest CT. Complications included acute respiratory distress syndrome (12 [29%]), RNAaemia (six [15%]), acute cardiac injury (five [12%]) and secondary infection (four [10%]). 13 (32%) patients were admitted to an ICU and six (15%)

died. Compared with non-ICU patients, ICU patients had higher plasma levels of IL2, IL7, IL10, GSCF, IP10, MCP1, MIP1A, and TNF alpha.

Interpretation The 2019-nCoV infection caused clusters of severe respiratory illness similar to severe acute respiratory syndrome coronavirus and was associated with ICU admission and high mortality. Major gaps in our knowledge of the origin, epidemiology, duration of human transmission, and clinical spectrum of disease need fulfilment by future studies. Copyright (C) 2020 Elsevier Ltd. All rights reserved.

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20 被引频次： 16360

题目： QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials

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Stefano); Fabris, S (Fabris, Stefano); Fratesi, G (Fratesi, Guido); Gebauer, R (Gebauer, Ralph); Gerstmann, U (Gerstmann, Uwe); Gougoussis, C (Gougoussis, Christos); Kokalj, A (Kokalj, Anton); Lazzeri, M (Lazzeri, Michele); Martin-Samos, L (Martin-Samos, Layla); Marzari, N (Marzari, Nicola); Mauri, F (Mauri, Francesco); Mazzarello, R (Mazzarello, Riccardo); Paolini, S (Paolini, Stefano); Pasquarello, A (Pasquarello, Alfredo); Paulatto, L (Paulatto, Lorenzo); Sbraccia, C (Sbraccia, Carlo); Scandolo, S (Scandolo, Sandro); Sclauzero, G (Sclauzero, Gabriele); Seitsonen, AP (Seitsonen, Ari P.); Smogunov, A (Smogunov, Alexander); Umari, P (Umari, Paolo); Wentzcovitch, RM (Wentzcovitch, Renata M.)

出处： JOURNAL OF PHYSICS-CONDENSED MATTER

摘要： QUANTUM ESPRESSO is an integrated suite of computer codes for electronic-structure calculations and materials modeling, based on density-functional theory, plane waves, and pseudopotentials (norm-conserving, ultrasoft, and projector-augmented wave). The acronym ESPRESSO stands for opEn Source Package for Research in Electronic Structure, Simulation, and Optimization. It is freely available to researchers around the world under the terms of the GNU General Public License. QUANTUM ESPRESSO builds upon newly-restructured electronic-structure codes that have been developed and tested by some of the original authors of novel electronic-structure algorithms and applied in the last twenty years by some of the leading materials modeling groups worldwide. Innovation and efficiency are still its main focus, with special attention paid to massively parallel architectures, and a great effort being devoted to user friendliness. QUANTUM ESPRESSO is evolving towards a distribution of independent and interoperable codes in the spirit of an open-source project, where researchers active in the field of electronic-structure calculations are encouraged to participate in the project by contributing their own codes or by implementing their own ideas into existing codes.

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21 被引频次： 16302
题目： Two-dimensional gas of massless Dirac fermions in graphene
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出处： NATURE
摘要: Quantum electrodynamics (resulting from the merger of quantum mechanics and relativity theory) has provided a clear understanding of phenomena ranging from particle physics to cosmology and from astrophysics to quantum chemistry(1-3). The ideas underlying quantum electrodynamics also influence the theory of condensed matter(4,5), but quantum relativistic effects are usually minute in the known experimental systems that can be described accurately by the non-relativistic Schrodinger equation. Here we report an experimental study of a condensed-matter system (graphene, a single atomic layer of carbon(6,7)) in which electron transport is essentially governed by Dirac's (relativistic) equation. The charge carriers in graphene mimic relativistic particles with zero rest mass and have an effective 'speed of light' c* approximate to 10(6) m s(-1). Our study reveals a variety of unusual phenomena that are characteristic of two-dimensional Dirac fermions. In particular we have observed the following: first, graphene's conductivity never falls below a minimum value corresponding to the quantum unit of conductance, even when concentrations of charge carriers tend to zero; second, the integer quantum Hall effect in graphene is anomalous in that it occurs at half-integer filling factors; and third, the cyclotron mass m(c) of massless carriers in graphene is described by E = m(c)c(*)(2). This two-dimensional system is not only interesting in itself but also allows access to the subtle and rich physics of quantum electrodynamics in a bench-top experiment.
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22 被引频次： 15837
题目： Single-crystal structure validation with the program PLATON
作者： Spek, AL (Spek, AL)
出处： JOURNAL OF APPLIED CRYSTALLOGRAPHY
摘要： The results of a single-crystal structure determination when in CIF format can now be validated routinely by automatic procedures. In this way, many errors in published papers can be avoided. The validation software generates a set of ALERTS detailing issues to be addressed by the experimenter, author, referee and publication journal. Validation was pioneered by the IUCr journal Acta Crystallographica Section C and is currently standard procedure for structures submitted for publication in all IUCr journals. The implementation of validation procedures by other journals is in progress. This paper describes the concepts of validation and the classes of checks that are carried out by the program PLATON as part of the IUCr checkCIF facility. PLATON validation can be run at any stage of the structure refinement, independent of the structure determination package used, and is recommended for use as a routine tool during or at least at the completion of every structure determination. Two examples are discussed where proper validation procedures could have avoided the publication of incorrect structures that had serious consequences for the chemistry involved.
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23 被引频次： 15298
题目： Features and development of Coot
作者： Emsley, P (Emsley, P.); Lohkamp, B (Lohkamp, B.); Scott, WG (Scott, W. G.); Cowtan, K (Cowtan, K.)
出处： ACTA CRYSTALLOGRAPHICA SECTION D-BIOLOGICAL CRYSTALLOGRAPHY
摘要： Coot is a molecular-graphics application for model building and validation of biological macromolecules. The program displays electron-density maps and atomic models and allows model manipulations such as idealization, real-space refinement, manual rotation/translation, rigid-body fitting, ligand search, solvation, mutations, rotamers and Ramachandran idealization. Furthermore, tools are provided for model validation as well as interfaces to external programs for refinement, validation and graphics. The software is designed to be easy to learn for novice users, which is achieved by ensuring that tools for common tasks are 'discoverable' through familiar user-interface elements (menus and toolbars) or by intuitive behaviour (mouse controls). Recent developments have focused on providing tools for expert users, with customisable key bindings, extensions and an extensive scripting interface. The software is under rapid development, but has already achieved very widespread use within the crystallographic community. The current state of the software is presented, with a description of the facilities available and of some of the underlying methods employed.
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24 被引频次： 15133
题目： THE ADSORPTION OF GASES ON PLANE SURFACES OF GLASS, MICA AND PLATINUM.
作者： Langmuir, I (Langmuir, Irving)
出处： JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
地址： Gen Elect Co, Res Lab, Schenectady, NY USA.

25 被引频次： 14952
题目： OLEX2: a complete structure solution, refinement and analysis program
作者： Dolomanov, OV (Dolomanov, Oleg V.); Bourhis, LJ (Bourhis, Luc J.); Gildea, RJ (Gildea, Richard J.); Howard, JAK (Howard, Judith A. K.); Puschmann, H (Puschmann, Horst
出处： JOURNAL OF APPLIED CRYSTALLOGRAPHY
摘要： New software, OLEX2, has been developed for the determination, visualization and analysis of molecular crystal structures. The software has a portable mouse-driven workflow-oriented and fully comprehensive graphical user interface for structure solution, refinement and report generation, as well as novel tools for structure analysis. OLEX2 seamlessly links all aspects of the structure solution, refinement and publication process and presents them in a single workflow-driven package, with the ultimate goal of producing an application which will be useful to both chemists and crystallographers.
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AIAA、IAF 最新会议

AIAA

（AIAA 来源：http://www.aiaa.org/）

1. **会议名称：**2022 Region I Student Conference
会议时间：25 March - 26 March 2022
会议地点：Hyatt Place, Blacksburg, Virginia, USA.
会议简介：Take part in AIAA's Regional Student Conference by presenting your research in a formal technical meeting, exchange ideas, and discuss programs with students from other universities in your region.
链接：
https://www.aiaa.org/events-learning/event/2022/03/25/default-calendar/2022-region-i-student-conference

2. **会议名称：**2022 Region III Student Conference
会议时间：25 March - 26 March 2022
会议地点：Neil Armstrong Hall of Engineering, Purdue University, West Lafayette, Indiana, USA
会议简介：Take part in AIAA's Regional Student Conference by presenting your research in a formal technical meeting, exchange ideas, and discuss programs with students from other universities in your region.
链接：
https://www.aiaa.org/events-learning/event/2022/03/25/default-calendar/2022-region-iii-student-conference

3. **会议名称：**2022 Region IV Student Conference
会议时间：1 April - 2 April 2022
会议地点：University of Texas at San Antonio, San Antonio, Texas, USA
会议简介：Take part in AIAA's Regional Student Conference by presenting your research in a formal technical meeting, exchange ideas, and discuss programs with students from other universities in your region.
链接：
https://www.aiaa.org/events-learning/event/2022/04/01/default-calendar/2022-region-iv-student-conference

4. **会议名称：**3rd International Academy of Astronautics (IAA) Conference on Space Situational Awareness
会议时间：4 April - 6 April 2022

会议地点：C/Santiago Grisolia, no. 4, Parque Tecnologico de Madrid (PTM), 28760 Tres Cantos, Madrid, Spain

会议简介：The 3rd IAA Conference on Space Situational Awareness will take place at C/Santiago Grisolia, no. 4, Parque Tecnologico de Madrid (PTM), Madrid, Spain, 4–6 April 2022.

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.

链接：

https://www.aiaa.org/events-learning/event/2022/04/04/default-calendar/3rd-international-academy-of-astronautics-(iaa)-conference-on-space-situational-awareness

5.会议名称：AIAA Aerospace Perspectives Series: Taking Advanced Computing to the Tactical Edge

会议时间：12 April 2022 1100 - 1200 (Eastern Daylight Time)

会议地点：Virtual

会议简介：Lockheed Martin is assembling an outstanding panel of industry and academic leaders to discuss taking edge computing technologies and capabilities to the tactical edge. Edge computing is a distributed computing topology where information processing is located close to the source of the information, bringing computation and data storage closer to the edge which is typically not done today. There are many commercial applications of edge computing and it is anticipated that there are a number of benefits to the defense battlespace. This webinar will seek to address what edge computing is – as it relates to defense applications, the defense capabilities that are enabled with edge computing, challenges and solutions associated with implementation, as well as defense-specific needs to successfully implement advanced computing capabilities at the tactical edge.

链接：

https://www.aiaa.org/events-learning/event/2022/04/12/default-calendar/aiaa-aerospace-perspectives-series-taking-advanced-computing-to-the-tactical-edge

IAF 最新会议

（IAF 来源：http://www.iafastro.org/）

会议名称：THE GLOBAL CONFERENCE ON SPACE FOR EMERGING COUNTRIES 2022
会议时间： 16 to 20 May 2022.
会议地点：Sideralis Foundation in Quito, Ecuador
会议简介：Creating awareness on the essential legislative and policy elements that must be considered in establishing a firm foundation for national or regional space programs;
Promoting the creation and development of a local space industry that is innovative, responsive, robust, commercially viable, and connected and integrated to the global space industry;
Highlighting the socio-economic benefits of space applications so that high-level citizen support can be secured for advancing national or regional space programs.
链接：
https://www.iafastro.org/events/global-series-conferences/the-global-conference-on-space-for-emerging-countries-2022/

ACM 最新会议

来源：http://www.acm.org/

1. **会议名称：**The 27th Annual International Conference On Mobile Computing And Networking
会议时间：March 28 - April 1, 2022
会议地点：New Orleans, United States
会议简介： ACM MobiCom 2021 is the twenty-seventh in a series of annual conferences sponsored by ACM SIGMOBILE dedicated to addressing the challenges in the areas of mobile computing and wireless and mobile networking. The MobiCom conference series serves as a highly selective, premier international forum addressing networks, systems, algorithms, and applications that support mobile computers and wireless networks. In addition to the regular conference program, MobiCom 2021 will include a set of workshops, research demonstrations, and a poster session that includes the ACM Student Research Competition.
链接：https://www.sigmobile.org/mobicom/2021/

2. **会议名称：**International Symposium on Physical Design
会议时间：Mar 27 - Mar 30, 2022
会议地点：Virtual Event, Canada
会议简介： The International Symposium on Physical Design provides a premier forum to exchange ideas and promote research on the physical design of VLSI systems. ISPD 2022 will feature state-of-the-art research from across the globe on traditional physical design topics related to ASIC and FPGA as well as emerging technologies in the area.
We will also pay tribute to Prof. Ricardo Reis (Federal University of Rio Grande do Sul, Brazil) for his instrumental impact on EDA research in South America and contributions to the physical design community.
链接：https://ispd.cc/ispd2022/index.php?page=home

3. **会议名称：** An Association of Computing Machinery (ACM) Special Interest Group on University and College Computing Services (SIGUCCS) Conference

会议时间：March 28, 2022 - April 8, 2022

会议地点：Online
会议简介：SIGUCCS is an Association for Computing Machinery (ACM) Special Interest Group on University and College Computing Services. SIGUCCS conference events and activities focus on the issues surrounding the support, delivery, and management of college and university information technology services. The conference format provides members and those in the field of college and university IT support a wide variety of learning and professional development opportunities.

链接：https://siguccs.org/Conference/2022/

4. 会议名称：Consortium for Computing Sciences in Colleges
会议时间：Apr 01 - Apr 02, 2022
会议地点：Springfield, USA
会议简介：As a proud member of the Consortium for Computing Sciences in Colleges, CCSC:Central Plains holds a yearly regional meeting enabling faculty from throughout the Central Plains area to gather to learn, network, and get energized about teaching and new developments in the Computing disciplines.
链接：https://www.ccsc.org/centralplains/

5. 会议名称：26th annual conference of the Consortium for Computing Sciences in Colleges Northeast Region
会议时间：April 1-2, 2022
会议地点：Pleasantville, USA
会议简介：The Consortium for Computing Sciences in Colleges Northeast Region (CCSCNE) brings together faculty, staff, and students from academic institutions throughout the northeastern U.S. and beyond to exchange ideas and information concerning undergraduate computing curricula.
链接：http://ccscne.org/conferences/ccscne-2022/

6. 会议名称：Principles and Practice of Parallel Programming 2022
会议时间：Apr 02 - Apr 06, 2022
会议地点：Seoul, Republic of Korea
会议简介：PPoPP is the premier forum for leading work on all aspects of parallel programming, including theoretical foundations, techniques, languages, compilers, runtime systems, tools, and practical experience. In the context of the symposium, “parallel programming” encompasses work on concurrent and parallel systems (multicore, multi-threaded, heterogeneous, clustered, and distributed systems; grids; datacenters; clouds; and large scale machines). Given the rise of parallel architectures in the consumer market (desktops, laptops, and mobile devices) and data centers, PPoPP is particularly interested in work that addresses new parallel workloads and issues that arise out of extreme-scale applications or cloud platforms, as well as techniques and tools that improve the productivity of parallel programming or work towards improved synergy with such emerging architectures.
链接：https://ppopp22.sigplan.org/

7. 会议名称：ACM SIGPLAN 2022 International Conference on Compiler Construction
会议时间：Apr 02 - Apr 03, 2022
会议地点：Seoul, USA
会议简介：The International Conference on Compiler Construction (CC) is interested in work on processing programs in the most general sense: analyzing, transforming or executing input that describes how a system operates, including traditional compiler construction as a special case.
链接：https://conf.researchr.org/home/CC-2022

8. 会议名称： The 27th Annual International Conference On Mobile Computing And Networking
会议时间：April 2nd - April 6th, 2022
会议地点：Seoul, South Korea
会议简介：The International Symposium on Code Generation and Optimization (CGO) provides a premier venue to bring together researchers and practitioners working at the interface of hardware and software on a wide range of optimization and code generation techniques and related issues. The conference spans the spectrum from purely static to fully dynamic approaches, and from pure software-based methods to specific architectural features and support for code generation and optimization.
链接：https://conf.researchr.org/home/cgo-2022

9. **会议名称：**19th USENIX Symposium on Networked Systems Design and Implementation
会议时间：APRIL 4–6, 2022
会议地点：RENTON, WA, USA
会议简介：Join us in Renton, WA, USA, on April 4–6, 2022, for the 19th USENIX Symposium on Networked Systems Design and Implementation. NSDI focuses on the design principles, implementation, and practical evaluation of networked and distributed systems. Our goal is to bring together researchers from across the networking and systems community to foster a broad approach to addressing overlapping research challenges.
链接：https://www.usenix.org/conference/nsdi22

10. **会议名称：**EuroSys conference
会议时间：Apr 05 - Apr 08, 2022
会议地点：RENNES, France
会议简介：EuroSys conference is a premier forum for discussing various issues of systems software research and development, including implications related to hardware and applications. The conference brings together professionals from academia and industry. It has a strong focus on systems research and development: operating systems, database systems, real-time systems, networked systems, storage systems, middleware, distributed, parallel, or embedded computing systems.
链接：https://2022.eurosys.org/

IQPC 最新国防会议(Defence)

IQPC 来源：http://www.iqpc.com/

1.会议名称： MILITARY FLIGHT TRAINING: EQUIPPING AIRCREW OF THE FUTURE
会议时间： 29 -31 March 2022
会议地点：London
会议简介：Military Flight Training 2022 will continue to discuss key challenge areas such as: 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.
Attracting over 250 military and industry attendees from over 40 nations, Military Flight Training 2022 arrives at a time where guaranteeing air superiority and strike capability has never been tougher.
链接：
https://www.defenceiq.com/events-militaryflighttrainginglondon?mac=DFIQ_Homepage_EOI_Title_Listing&utm_medium=Portal&utm_source=defence-iq

2.会议名称：Securing the Defence Industrial Base: Mitigating Risk and Delivering Resiliency in Physical and Digital Supply Chains
会议时间：21 April, 2022
会议地点： Online
会议简介：The Influence major disruptions have had on the identification of risks across the DIB supply chain
Ongoing efforts to strengthen the defense industrial base to mitigate short- and long-term risk
Recent Government and Military initiatives being introduced to help the advancement of regional suppliers
How these initiatives will influence the entire supply chain
Ways to build trustworthy supply chain networks to maintain business continuity and gain a competitive advantage
The impact policy changes and regulations are having across America
From acquisition process to compliance, debating the policy, process, and practical governmental initiatives the defense sector needs to facilitate resilient supply chains.
链接：
https://www.defenceiq.com/defence-technology/webinars/interos?mac=DFIQ_Homepage_EOI_Title_Listing&utm_medium=Portal&utm_source=defence-iq_

3.会议名称：Wildfire Management Summit 2022
会议时间：April 25-26, 2022
会议地点：San Francisco, CA
会议简介：In the face of a changing climate and the increased frequency and power of wildfires, the need to effectively mitigate and manage their start and spread has grown more and more evident. There is a persistent need for emergency managers and firefighters across the United States and the world to be prepared and equipped to respond effectively to the latest disasters to prevent casualties and damage to property, infrastructure and ecosystems.
链接：
https://www.idga.org/events-wildfiremanagement?mac=DFIQ_Homepage_EOI_Title_Listing&utm_medium=Portal&utm_source=defence-iq

4.会议名称：The Global Intelligence and C2 Community's Annual General Meeting
会议时间：26 - 29 April, 2022
会议地点：Leonardo Royal St Paul's, London, UK
会议简介：elcoming over 250 senior decision-makers, C2ISR Week integrates the Airborne, Maritime and Land C2ISR conferences to provide a forum for discussions on ways to transform intelligence for future all domain warfare. Benefiting from the personal interventions of Lt Gen Rouleaou, Lt Gen Crall, and Lt Gen Berrier and many other senior decision-makers, the previous event explored, amongst other themes, the operationalization of JADC2 and AFSC, distributed decision-making (mission command) in degraded and denied environments, and the role of the airborne platform within next-generation C2ISR.
链接：
https://www.defenceiq.com/events-c2isrweek?mac=DFIQ_Homepage_EOI_Title_Listing&utm_medium=Portal&utm_source=defence-iq

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