Science Newsletter

2023 Volume 4 (Total 32) *Website:http://lib.jsut.edu.cn/2018/1015/c5474a113860/page.htm*
September, 2022

Contents

Editor: Chaoyi Chu（褚朝奕） TEL: 3548 Email: ccy@jsut.edu.cn

Introduction:

There are 3 main elements in the Science Newsletter which is composed. In the first part, we list the most up to date papers about central issues for each discipline in our university, and they are provided with 5 subjects for a time. In the second part, there are papers from the top journals last month, and most of them are from Nature and Science. In the third part, we post information about calling papers for international conferences. Hopefully, some of the information in this manuscript may be useful for those who are dedicating to scientific career. Besides, the journals are also posted on the website of our library, and they are available to be accessed any time at https://lib.jsut.edu.cn/2018/1015/c5474a113860/page.htm . If there are any questions or suggestions, please send e-mails to ccy@jsut.edu.cn in no hesitate.

Ⅰ Topics

The keywords of this month is **Computer Science**:
We list several papers which are related to the top concerned topics in computer science researches. The papers are classified in 5 categories, and they are: **Machine Learning Algorithms, Neural Networks, Deep Learning, Natural Language Processing,** and **Pattern Recognition**. Also, the listed papers are all arranged in a descending sort of impact factor, and there are also accesses right after each abstract of papers. Last but not least, the papers from ~~**predatory journals**~~ are excluded for a better academic environment.

MACHINE LEARNING ALGORITHMS

IEEE Trans Pattern Anal Mach Intell (impact factor: 23.6) 1 区 TOP

Regularized Optimal Transport Layers for Generalized Global Pooling Operations.

Xu, Cheng, et. al

Abstract:

Global pooling is one of the most significant operations in many machine learning models and tasks, which works for information fusion and structured data (like sets and

Editor: Chaoyi Chu（褚朝奕） TEL: 3548 Email: ccy@jsut.edu.cn

graphs) representation. However, without solid mathematical fundamentals, its practical implementations often depend on empirical mechanisms and thus lead to sub-optimal, even unsatisfactory performance. In this work, we develop a novel and generalized global pooling framework through the lens of optimal transport. The proposed framework is interpretable from the perspective of expectation-maximization. Essentially, it aims at learning an optimal transport across sample indices and feature dimensions, making the corresponding pooling operation maximize the conditional expectation of input data. We demonstrate that most existing pooling methods are equivalent to solving a regularized optimal transport (ROT) problem with different specializations, and more sophisticated pooling operations can be implemented by hierarchically solving multiple ROT problems. Making the parameters of the ROT problem learnable, we develop a family of regularized optimal transport pooling (ROTP) layers. We implement the ROTP layers as a new kind of deep implicit layer. Their model architectures correspond to different optimization algorithms. We test our ROTP layers in several representative set-level machine learning scenarios, including multi-instance learning (MIL), graph classification, graph set representation, and image classification. Experimental results show that applying our ROTP layers can reduce the difficulty of the design and selection of global pooling - our ROTP layers may either imitate some existing global pooling methods or lead to some new pooling layers fitting data better. The code is available at https://github.com/SDS-Lab/ROT-Pooling.

Anal Chem (impact factor: 7.4) 2 区 TOP

Machine Learning Analysis of Raman Spectra To Quantify the Organic Constituents in Complex Organic-Mineral Mixtures

Zarei, Solomatova, et. al

Abstract:

Important decisions in local agricultural policy and practice often hinge on the soil's chemical composition. Raman spectroscopy offers a rapid noninvasive means to quantify the constituents of complex organic systems. But the application of Raman spectroscopy to soils presents a multifaceted challenge due to organic/mineral compositional complexity and spectral interference arising from overwhelming fluorescence. The present work compares methodologies with the capacity to help overcome common obstacles that arise in the analysis of soils. We created conditions representative of these challenges by combining varying proportions of six amino acids commonly found in soils with fluorescent bentonite clay and coarse mineral components. Referring to an extensive data set of Raman spectra, we compare the performance of the convolutional neural network (CNN) and partial least-squares regression (PLSR) multivariate models for amino acid composition. Strategies employing volume-averaged spectral sampling and data preprocessing algorithms improve the predictive power of these models. Our average test R2 for PLSR models exceeds 0.89 and approaches 0.98, depending on the complexity of the matrix, whereas

CNN yields an R2 range from 0.91 to 0.97, demonstrating that classic PLSR and CNN perform comparably, except in cases where the signal-to-noise ratio of the organic component is very low, whereupon CNN models outperform. Artificially isolating two of the most prevalent obstacles in evaluating the Raman spectra of soils, we have characterized the effect of each obstacle on the performance of machine learning models in the absence of other complexities. These results highlight important considerations and modeling strategies necessary to improve the Raman analysis of organic compounds in complex mixtures in the presence of mineral spectral components and significant fluorescence.

Nephrol Dial Transplant (impact factor: 6.1) 2 ☒

Urinary peptidomic liquid biopsy for non-invasive differential diagnosis of chronic kidney disease.

Mavrogeorgis, He, et. al

Abstract:

Specific urinary peptides hold information on disease pathophysiology, which, in combination with artificial intelligence (AI), could enable non-invasive assessment of chronic kidney disease (CKD) aetiology. Existing approaches are generally specific for the diagnosis of single aetiologies. We present the development of models able to simultaneously distinguish and spatially visualize multiple CKD aetiologies.The urinary peptide data of 1850 healthy control (HC) and CKD (diabetic kidney disease-DKD, IgA nephropathy-IgAN, and vasculitis) participants was extracted from the Human Urinary Proteome Database. Uniform manifold approximation and projection (UMAP) coupled to a support vector machine (SVM) algorithm was used to generate multidimensional peptide models to perform binary (DKD versus HC) and multiclass (DKD, HC, IgAN, vasculitis) classifications. This pipeline was compared to the current state-of-the-art of single aetiology CKD urinary peptide models.In an independent test set, the developed models achieved 90.35% and 70.13% overall predictive accuracies, respectively, for the binary and the multiclass classifications. Omitting the UMAP step led to improved predictive accuracies (96.14% and 85.06%, respectively). As expected, the HC class was distinguished with the highest accuracy. The different classes displayed a tendency to form distinct clusters in the 3D-space based on their disease state.Urinary peptide data present an effective basis for CKD aetiology differentiation using machine learning models. Although adding the UMAP step to the models did not improve prediction accuracy, it may provide a unique visualization advantage. Additional studies are warranted to further validate the pipeline's clinical potential as well as expand to other CKD aetiologies and also other diseases.© The Author(s) 2023. Published by Oxford University Press on behalf of the ERA.

Adv Mater (impact factor: 29.4) 1 区 TOP

Machine Learning Paves the Way for High Entropy Compounds Exploration: Challenges, Progress, and Outlook.

Wan, Li, Yu, et. al

Abstract:
Machine learning (ML) has emerged as a powerful tool in the research field of high entropy compounds (HEC), which have gained worldwide attention due to their vast compositional space and abundant regulatability. However, the complex structure space of HEC poses challenges to traditional experimental and computational approaches, necessitating the adoption of machine learning. Microscopically, machine learning can model the Hamiltonian of the HEC system, enabling atomic-level property investigations, while macroscopically, it can analyze macroscopic material characteristics such as hardness, melting point, and ductility. Various machine learning algorithms, both traditional methods and deep neural networks can be employed in HEC research. Comprehensive and accurate data collection, feature engineering, and model training and selection through cross-validation are crucial for establishing excellent ML models. ML also holds promise in analyzing phase structures and stability, constructing potentials in simulations, and facilitating the design of functional materials. Although some domains, such as magnetic and device materials, still require further exploration, machine learning's potential in HEC research is substantial. Consequently, machine learning has become an indispensable tool in understanding and exploiting the capabilities of HEC, serving as the foundation for the new paradigm of artificial intelligence-assisted material exploration. This article is protected by copyright. All rights reserved.This article is protected by copyright. All rights reserved.

J Environ Manage (impact factor: 8.7) 2 区

Forecasting actual evapotranspiration without climate data based on stacked integration of DNN and meta-heuristic models across China from 1958 to 2021.

Elbeltagi, Srivastava, et al

Abstract:
As a non-linear phenomenon that varies along with agro-climatic conditions alongside many other factors, Evapotranspiration (ET) process represents a complexity when be assessed especially if there is a data scarcity in the weather data. However, even under such a data scarcity, the accurate estimates of ET values remain necessary for precise irrigation. So, the present study aims to: i) evaluate the performance of six hybrid machine learning (ML) models in estimating the monthly actual ET values under

different agro-climatic conditions in China for seven provinces (Shandong, Jiangsu, Zhejiang, Fujian, Jiangxi, Hubei, and Henan), and ii) select the best-developed model based on statistical metrics and reduce errors between predicted and actual ET (AET) values. AET datasets were divided into 78% for model training (from 1958 to 2007) and the remaining was used for testing (from 2008 to 2021). Deep Neural Networks (DNN) was used as a standalone model at first then the stacking method was applied to integrate DNN with data-driven models such as Additive regression (AR), Random Forest (RF), Random Subspace (RSS), M5 Burned Tree (M5P) and Reduced Error Purning Tree (REPTree). Partial Auto-Correlation Function (PACF) was used for selection of the best lags inputs to the developed models. Results have revealed that DNN-based hybrid models held better performance than non-hybrid DNN models, such that the DNN-RF algorithm outperformed others during both training and testing stages, followed by DNN-RSS. This model has acquired the best values of every statistical measure [MAE (10.8, 12.9), RMSE (15.6, 17.4), RAE (31.9%, 41.4%), and RRSE (39.3%, 47.2%)] for training and testing, respectively. In contrast, the DNN model held the worst performance [MAE (14.9, 13.7), RMSE (20.1, 18.2), RAE (43.9%, 43.7%), and RRSE (50.6%, 49.3%)], for training and testing, respectively. Results from the study presented have revealed the capability of DNN-based hybrid models for long-term predictions of the AET values. Moreover, the DNN-RF model has been suggested as the most suitable model to improve future investigation for AET predictions, which could benefit the enhancement of the irrigation process and increase crop yield.

J Environ Manage (impact factor: 8.7) 2 ☒

A multi-tier deterioration assessment models for sewer and stormwater pipelines in Hong Kong.

Abdelkhalek, Zayed, et. al

Abstract:

Sewerage and stormwater networks are subjected to several deterioration factors, including aging, environmental conditions, and traffic. Maintaining these critical assets in good condition is essential to avoid harmful consequences, such as environmental contamination and negative implications on other infrastructure systems (e.g., water and road networks). Deterioration assessment models are effective and cost-efficient means for proactive management systems that can reduce such consequences. In this connection, this study aims to develop deterioration assessment models for sewer and stormwater pipelines in Hong Kong. First, critical factors that impact the deterioration process of these pipelines were identified. Data for these factors were then collected from the Drainage Services Department (DSD) and open-source data provided by the Hong Kong government. To improve prediction accuracy, a multi-tier concept was utilized in building the models. The first tier categorized pipelines into two groups: fail and not fail, whereas the second tier

assigned a grade range from 1 to 3 to the "not fail" pipelines. Several artificial intelligence approaches, such as random forest, neural network, and SVM, were tested. Random forest achieved the highest accuracy in predicting pipelines condition, followed by neural networks. A sensitivity analysis was carried out to investigate the combined impact of two factors, with age being one of them, on the pipeline's performance. The findings of this study provide a robust decision-making tool that DSD authorities and consultants can use to optimize inspection and maintenance activities.

DEEP LEARNING

ACS Nano (impact factor: 17.1) 1 区 TOP

Deep Learning Assisted Surface-Enhanced Raman Spectroscopy (SERS) for Rapid and Direct Nucleic Acid Amplification and Detection: Toward Enhanced Molecular Diagnostics.

Kim, Jue, Lee, et. al

Abstract:
Surface-enhanced Raman scattering (SERS) has evolved into a robust analytical technique capable of detecting a variety of biomolecules despite challenges in securing a reliable Raman signal. Conventional SERS-based nucleic acid detection relies on hybridization assays, but reproducibility and signal strength issues have hindered research on directly amplifying nucleic acids on SERS surfaces. This study introduces a deep learning assisted ZnO-Au-SERS-based direct amplification (ZADA) system for rapid, sensitive molecular diagnostics. The system employs a SERS substrate fabricated by depositing gold on uniformly grown ZnO nanorods. These nanorods create hot spots for the amplification of the target nucleic acids directly on the SERS surface, eliminating the need for postamplification hybridization and Raman reporters. The limit of detection of the ZADA system was superior to those of the conventional amplification methods. Clinical validation of the ZADA system with coronavirus disease 2019 (COVID-19) samples from human patients yielded a sensitivity and specificity of 92.31% and 81.25%, respectively. The integration of a deep learning program further enhanced sensitivity and specificity to 100% and reduced SERS analysis time, showcasing the potential of the ZADA system for rapid, label-free disease diagnosis via direct nucleic acid amplification and detection within 20 min.

Editor: Chaoyi Chu（褚朝奕） TEL: 3548 Email: ccy@jsut.edu.cn

IEEE Trans Neural Netw Learn Syst (impact factor: 10.4) 1 区 TOP

Rectify ViT Shortcut Learning by Visual Saliency.

Ma, Zhao, Chen, et. al

Abstract:

Shortcut learning in deep learning models occurs when unintended features are prioritized, resulting in degenerated feature representations and reduced generalizability and interpretability. However, shortcut learning in the widely used vision transformer (ViT) framework is largely unknown. Meanwhile, introducing domain-specific knowledge is a major approach to rectifying the shortcuts that are predominated by background-related factors. For example, eye-gaze data from radiologists are effective human visual prior knowledge that has the great potential to guide the deep learning models to focus on meaningful foreground regions. However, obtaining eye-gaze data can still sometimes be time-consuming, labor-intensive, and even impractical. In this work, we propose a novel and effective saliency-guided ViT (SGT) model to rectify shortcut learning in ViT with the absence of eye-gaze data. Specifically, a computational visual saliency model (either pretrained or fine-tuned) is adopted to predict saliency maps for input image samples. Then, the saliency maps are used to filter the most informative image patches. Considering that this filter operation may lead to global information loss, we further introduce a residual connection that calculates the self-attention across all the image patches. The experiment results on natural and medical image datasets show that our SGT framework can effectively learn and leverage human prior knowledge without eye-gaze data and achieves much better performance than baselines. Meanwhile, it successfully rectifies the harmful shortcut learning and significantly improves the interpretability of the ViT model, demonstrating the promise of transferring human prior knowledge derived visual saliency in rectifying shortcut learning.

IEEE J Biomed Health Inform (impact factor: 7.7) 2 区

Fusion-Based Deep Learning Architecture for Detecting Drug-Target Binding Affinity Using Target and Drug Sequence and Structure.

Wang, Li, et. al

Abstract:

Accurately predicting drug-target binding affinity plays a vital role in accelerating drug discovery. Many computational approaches have been proposed due to costly and time-consuming of wet laboratory experiments. In the input representation, most methods only focus on the target sequence properties or target structure properties while ignore the overall contribution. Therefore, we develop a novel fusion protocol based on multiscale convolutional neural networks and graph neural networks, named CGraphDTA, to predict drug-target binding affinity using target sequence and structure.

Unlike existing methods, CGraphDTA is the first model constructed with target sequence and structure as input. Concretely, the multiscale convolutional neural networks are utilized to extract target and drug presentation from sequence, graph neuralnetworksareemployedtoextractgraphpresentation from target and drug molecular structure. We compare CGraphDTA with the state-of-the-art methods, the results show that our model outperforms the current methods on the test sets. Furthermore, we conduct ablation studies, biological interpretation examination and drug selectivity evaluation, all results suggest that CGraphDTA is a useful tool to predict drug-target binding affinity and accelerate drug discovery. The resource codes are available at https://github.com/CSUBioGroup/CGraphDTA.

NATURAL LANGUAGE PROCESSING

JAMA Netw Open (impact factor: 13.8) 2 ☒

Video Intervention and Goals-of-Care Documentation in Hospitalized Older Adults: The VIDEO-PCE Randomized Clinical Trial.

Volandes, Zupanc, et. al

Abstract

Despite the benefits of goals-of-care (GOC) communication, many hospitalized individuals never communicate their goals or preferences to clinicians.To assess whether a GOC video intervention delivered by palliative care educators (PCEs) increased the rate of GOC documentation.This pragmatic, stepped-wedge cluster randomized clinical trial included patients aged 65 years or older admitted to 1 of 14 units at 2 urban hospitals in New York and Boston from July 1, 2021, to October 31, 2022.The intervention involved PCEs (social workers and nurses trained in GOC communication) facilitating GOC conversations with patients and/or their decision-makers using a library of brief, certified video decision aids available in 29 languages. Patients in the control period received usual care.The primary outcome was GOC documentation, which included any documentation of a goals conversation, limitation of life-sustaining treatment, palliative care, hospice, or time-limited trials and was obtained by natural language processing.A total of 10 802 patients (mean [SD] age, 78 [8] years; 51.6% male) were admitted to 1 of 14 hospital units. Goals-of-care documentation during the intervention phase occurred among 3744 of 6023 patients (62.2%) compared with 2396 of 4779 patients (50.1%) in the usual care phase ($P < .001$). Proportions of documented GOC discussions for Black or African American individuals (865 of 1376 [62.9%] vs 596 of 1125 [53.0%]), Hispanic or Latino individuals (311 of 548 [56.8%] vs 218 of 451 [48.3%]), non-English speakers (586 of 1059 [55.3%] vs 405 of 863 [46.9%]), and people living with Alzheimer

disease and related dementias (520 of 681 [76.4%] vs 355 of 570 [62.3%]) were greater during the intervention phase compared with the usual care phase.In this stepped-wedge cluster randomized clinical trial of older adults, a GOC video intervention delivered by PCEs resulted in higher rates of GOC documentation compared with usual care, including among Black or African American individuals, Hispanic or Latino individuals, non-English speakers, and people living with Alzheimer disease and related dementias. The findings suggest that this form of patient-centered care delivery may be a beneficial decision support tool.ClinicalTrials.gov Identifier: NCT04857060.

J Cheminform (impact factor: 8.6) 2 区 TOP

pyPept: a python library to generate atomistic 2D and 3D representations of peptides

Rodrigo Ochoa, J. B. Brown, et. al

Abstract

We present pyPept, a set of executables and underlying python-language classes to easily create, manipulate, and analyze peptide molecules using the FASTA, HELM, or recently-developed BILN notations. The framework enables the analysis of both pure proteinogenic peptides as well as those with non-natural amino acids, including support to assemble a customizable monomer library, without requiring programming. From line notations, a peptide is transformed into a molecular graph for 2D depiction tasks, the calculation of physicochemical properties, and other systematic analyses or processing pipelines. The package includes a module to rapidly generate approximate peptide conformers by incorporating secondary structure restraints either given by the user or predicted via pyPept, and a wrapper tool is also provided to automate the generation and output of 2D and 3D representations of a peptide directly from the line notation. HELM and BILN notations that include circular, branched, or stapled peptides are fully supported, eliminating errors in structure creation that are prone during manual drawing and connecting. The framework and common workflows followed in pyPept are described together with illustrative examples. pyPept has been released at: https://github.com/Boehringer-Ingelheim/pyPept.

ACS Synth Biol (impact factor: 4.7) 2 区

Statistical Analysis and Tokenization of Epitopes to Construct Artificial Neoepitope Libraries.

Lopez-Martinez, Manteca, et. al

Abstract

Epitopes are specific regions on an antigen's surface that the immune system recognizes. Epitopes are usually protein regions on foreign immune-stimulating entities such as

viruses and bacteria, and in some cases, endogenous proteins may act as antigens. Identifying epitopes is crucial for accelerating the development of vaccines and immunotherapies. However, mapping epitopes in pathogen proteomes is challenging using conventional methods. Screening artificial neoepitope libraries against antibodies can overcome this issue. Here, we applied conventional sequence analysis and methods inspired in natural language processing to reveal specific sequence patterns in the linear epitopes deposited in the Immune Epitope Database (www.iedb.org) that can serve as building blocks for the design of universal epitope libraries. Our results reveal that amino acid frequency in annotated linear epitopes differs from that in the human proteome. Aromatic residues are overrepresented, while the presence of cysteines is practically null in epitopes. Byte pair encoding tokenization shows high frequencies of tryptophan in tokens of 5, 6, and 7 amino acids, corroborating the findings of the conventional sequence analysis. These results can be applied to reduce the diversity of linear epitope libraries by orders of magnitude.

PATTERN RECOGNITION

Nat Rev Rheumatol (impact factor: 33.7) 1 区 TOP

Imaging in inflammatory arthritis: progress towards precision medicine.

Minopoulou, Kleyer, et. al

Abstract

Imaging techniques such as ultrasonography and MRI have gained ground in the diagnosis and management of inflammatory arthritis, as these imaging modalities allow a sensitive assessment of musculoskeletal inflammation and damage. However, these techniques cannot discriminate between disease subsets and are currently unable to deliver an accurate prediction of disease progression and therapeutic response in individual patients. This major shortcoming of today's technology hinders a targeted and personalized patient management approach. Technological advances in the areas of high-resolution imaging (for example, high-resolution peripheral quantitative computed tomography and ultra-high field MRI), functional and molecular-based imaging (such as chemical exchange saturation transfer MRI, positron emission tomography, fluorescence optical imaging, optoacoustic imaging and contrast-enhanced ultrasonography) and artificial intelligence-based data analysis could help to tackle these challenges. These new imaging approaches offer detailed anatomical delineation and an in vivo and non-invasive evaluation of the immunometabolic status of inflammatory reactions, thereby facilitating an in-depth characterization of inflammation. By means of these developments, the aim of earlier diagnosis, enhanced monitoring and, ultimately, a personalized treatment strategy looms closer.© 2023.

Springer Nature Limited.

Trends Immunol (impact factor: 16.8) 1 区 TOP

Carbohydrates as putative pattern recognition receptor agonists in vaccine development.

Mu, Dong, et. al

Abstract:
Adjuvants are essential components of modern vaccines. One general mechanism underlying their immunostimulatory functions is the activation of pattern recognition receptors (PRRs) of innate immune cells. Carbohydrates - as essential signaling molecules on microbial surfaces - are potent PRR agonists and candidate materials for adjuvant design. Here, we summarize the latest trends in developing carbohydrate-containing adjuvants, with fresh opinions on how the physicochemical characteristics of the glycans (e.g., molecular size, assembly status, monosaccharide components, and functional group patterns) affect their adjuvant activities in aiding antigen transport, regulating antigen processing, and enhancing adaptive immune responses. From a translational perspective, we also discuss potential technologies for solving long-lasting challenges in carbohydrate adjuvant design.

Food Chem (impact factor: 8.8) 2 区 TOP

Machine learning-assisted fluorescence sensor array for qualitative and quantitative analysis of pyrethroid pesticides.

Li, Pan, et. al

Abstract:
The simultaneous detection of multiple residues of pyrethroid pesticides (PPs) on vegetables and fruits is still challenging using traditional nanosensing methods due to the high structural similarity of PPs. In this work, sensor arrays composed of three nanocomposite complexes (rhodamine B-CD@Au, rhodamine 6G-CD@Au, and coumarin 6-CD@Au) were constructed to discriminate between structurally similar PPs. Four PPs, deltamethrin, fenvalerate, cyfluthrin, and fenpropathrin, were successfully discriminated. The ability of these sensor units was derived from the different affinity between receptor/analyte and receptor/dye, as well as the non-linear relationship between fluorescence signal and analyte concentration. Upon multivariate pattern recognition analysis, the array performed high-throughput identification of four PPs in unknown samples with 100% classification accuracy. In addition, good accuracy of predicting concentration using the "stepwise prediction" strategy combined with the machine learning method was achieved.

Editor: Chaoyi Chu（褚朝奕） TEL: 3548 Email: ccy@jsut.edu.cn

Ⅱ Concentration

PHYSICS

No thick carbon dioxide atmosphere on the rocky exoplanet TRAPPIST-1 c

Zieba, Sebastian, et al.

Abstract

Seven rocky planets orbit the nearby dwarf star TRAPPIST-1, providing a unique opportunity to search for atmospheres on small planets outside the Solar System[1]. Thanks to the recent launch of the James Webb Space Telescope (JWST), possible atmospheric constituents such as carbon dioxide (CO_2) are now detectable[2,3]. Recent JWST observations of the innermost planet TRAPPIST-1 b showed that it is most probably a bare rock without any CO_2 in its atmosphere[4]. Here we report the detection of thermal emission from the dayside of TRAPPIST-1 c with the Mid-Infrared Instrument (MIRI) on JWST at 15 μm. We measure a planet-to-star flux ratio of $f_p/f_* = 421 \pm 94$ parts per million (ppm), which corresponds to an inferred dayside brightness temperature of 380 ± 31 K. This high dayside temperature disfavours a thick, CO_2-rich atmosphere on the planet. The data rule out cloud-free O_2/CO_2 mixtures with surface pressures ranging from 10 bar (with 10 ppm CO_2) to 0.1 bar (pure CO_2). A Venus-analogue atmosphere with sulfuric acid clouds is also disfavoured at 2.6σ confidence. Thinner atmospheres or bare-rock surfaces are consistent with our measured planet-to-star flux ratio. The absence of a thick, CO_2-rich atmosphere on TRAPPIST-1 c suggests a relatively volatile-poor formation history, with less than \({9.5}_{-2.3}^{+7.5}\) Earth oceans of water. If all planets in the system formed in the same way, this would indicate a limited reservoir of volatiles for the potentially habitable planets in the system.

Spin–vibronic coherence drives singlet–triplet conversion

Rafiq, Shahnawaz, et al.

Abstract

Design-specific control over the transitions between excited electronic states with different spin multiplicities is of the utmost importance in molecular and materials chemistry1,2,3. Previous studies have indicated that the combination of spin–orbit and vibronic effects, collectively termed the spin–vibronic effect, can accelerate quantum-mechanically forbidden transitions at non-adiabatic crossings4,5. However, it has been difficult to identify precise experimental manifestations of the spin–vibronic

mechanism. Here we present coherence spectroscopy experiments that reveal the interplay between the spin, electronic and vibrational degrees of freedom that drive efficient singlet–triplet conversion in four structurally related dinuclear Pt(II) metal–metal-to-ligand charge-transfer (MMLCT) complexes. Photoexcitation activates the formation of a Pt–Pt bond, launching a stretching vibrational wavepacket. The molecular-structure-dependent decoherence and recoherence dynamics of this wavepacket resolve the spin–vibronic mechanism. We find that vectorial motion along the Pt–Pt stretching coordinates tunes the singlet and intermediate-state energy gap irreversibly towards the conical intersection and subsequently drives formation of the lowest stable triplet state in a ratcheting fashion. This work demonstrates the viability of using vibronic coherences as probes6,7,8,9 to clarify the interplay among spin, electronic and nuclear dynamics in spin-conversion processes, and this could inspire new modular designs to tailor the properties of excited states.

First observation of 28O

Kondo, Y., Achouri, N. L., et al.

Abstract

Subjecting a physical system to extreme conditions is one of the means often used to obtain a better understanding and deeper insight into its organization and structure. In the case of the atomic nucleus, one such approach is to investigate isotopes that have very different neutron-to-proton (N/Z) ratios than in stable nuclei. Light, neutron-rich isotopes exhibit the most asymmetric N/Z ratios and those lying beyond the limits of binding, which undergo spontaneous neutron emission and exist only as very short-lived resonances (about 10^{-21} s), provide the most stringent tests of modern nuclear-structure theories. Here we report on the first observation of ^{28}O and ^{27}O through their decay into ^{24}O and four and three neutrons, respectively. The ^{28}O nucleus is of particular interest as, with the $Z = 8$ and $N = 20$ magic numbers[1,2], it is expected in the standard shell-model picture of nuclear structure to be one of a relatively small number of so-called 'doubly magic' nuclei. Both ^{27}O and ^{28}O were found to exist as narrow, low-lying resonances and their decay energies are compared here to the results of sophisticated theoretical modelling, including a large-scale shell-model calculation and a newly developed statistical approach. In both cases, the underlying nuclear interactions were derived from effective field theories of quantum chromodynamics. Finally, it is shown that the cross-section for the production of ^{28}O from a ^{29}F beam is consistent with it not exhibiting a closed $N = 20$ shell structure.

Spin-mediated shear oscillators in a van der Waals antiferromagnet

Zong, Alfred, et al.

Abstract

Understanding how microscopic spin configuration gives rise to exotic properties at the macroscopic length scale has long been pursued in magnetic materials[1,2,3,4,5]. One seminal example is the Einstein–de Haas effect in ferromagnets[1,6,7], in which angular momentum of spins can be converted into mechanical rotation of an entire object. However, for antiferromagnets without net magnetic moment, how spin ordering couples to macroscopic movement remains elusive. Here we observed a seesaw-like rotation of reciprocal lattice peaks of an antiferromagnetic nanolayer film, whose gigahertz structural resonance exhibits more than an order-of-magnitude amplification after cooling below the Néel temperature. Using a suite of ultrafast diffraction and microscopy techniques, we directly visualize this spin-driven rotation in reciprocal space at the nanoscale. This motion corresponds to interlayer shear in real space, in which individual micro-patches of the film behave as coherent oscillators that are phase-locked and shear along the same in-plane axis. Using time-resolved optical polarimetry, we further show that the enhanced mechanical response strongly correlates with ultrafast demagnetization, which releases elastic energy stored in local strain gradients to drive the oscillators. Our work not only offers the first microscopic view of spin-mediated mechanical motion of an antiferromagnet but it also identifies a new route towards realizing high-frequency resonators[8,9] up to the millimetre band, so the capability of controlling magnetic states on the ultrafast timescale[10,11,12,13] can be readily transferred to engineering the mechanical properties of nanodevices.

All-perovskite tandem solar cells with 3D/3D bilayer perovskite heterojunction

Lin, Renxing, et al.

Abstract

All-perovskite tandem solar cells promise higher power-conversion efficiency (PCE) than single-junction perovskite solar cells (PSCs) while maintaining a low fabrication cost1,2,3. However, their performance is still largely constrained by the subpar performance of mixed lead–tin (Pb–Sn) narrow-bandgap (NBG) perovskite subcells, mainly because of a high trap density on the perovskite film surface4,5,6. Although heterojunctions with intermixed 2D/3D perovskites could reduce surface recombination, this common strategy induces transport losses and thereby limits device fill factors (FFs)7,8,9. Here we develop an immiscible 3D/3D bilayer perovskite heterojunction

(PHJ) with type II band structure at the Pb–Sn perovskite–electron-transport layer (ETL) interface to suppress the interfacial non-radiative recombination and facilitate charge extraction. The bilayer PHJ is formed by depositing a layer of lead-halide wide-bandgap (WBG) perovskite on top of the mixed Pb–Sn NBG perovskite through a hybrid evaporation–solution-processing method. This heterostructure allows us to increase the PCE of Pb–Sn PSCs having a 1.2-μm-thick absorber to 23.8%, together with a high open-circuit voltage (Voc) of 0.873 V and a high FF of 82.6%. We thereby demonstrate a record-high PCE of 28.5% (certified 28.0%) in all-perovskite tandem solar cells. The encapsulated tandem devices retain more than 90% of their initial performance after 600 h of continuous operation under simulated one-sun illumination.

Mixed-dimensional moiré systems of twisted graphitic thin films

Waters, Dacen, et al.

Abstract

Moiré patterns formed by stacking atomically thin van der Waals crystals with a relative twist angle can give rise to notable new physical properties1,2. The study of moiré materials has so far been limited to structures comprising no more than a few van der Waals sheets, because a moiré pattern localized to a single two-dimensional interface is generally assumed to be incapable of appreciably modifying the properties of a bulk three-dimensional crystal. Here, we perform transport measurements of dual-gated devices constructed by slightly rotating a monolayer graphene sheet atop a thin bulk graphite crystal. We find that the moiré potential transforms the electronic properties of the entire bulk graphitic thin film. At zero and in small magnetic fields, transport is mediated by a combination of gate-tuneable moiré and graphite surface states, as well as coexisting semimetallic bulk states that do not respond to gating. At high field, the moiré potential hybridizes with the graphitic bulk states due to the unique properties of the two lowest Landau bands of graphite. These Landau bands facilitate the formation of a single quasi-two-dimensional hybrid structure in which the moiré and bulk graphite states are inextricably mixed. Our results establish twisted graphene–graphite as the first in a new class of mixed-dimensional moiré materials.

CHEMISTRY

A machine-learning tool to predict substrate-adaptive conditions for Pd-catalyzed C–N couplings

N. Ian Rinehart, Rakesh K. Saunthwal, et. al

Abstract

Machine-learning methods have great potential to accelerate the identification of reaction conditions for chemical transformations. A tool that gives substrate-adaptive conditions for palladium (Pd)–catalyzed carbon-nitrogen (C–N) couplings is presented. The design and construction of this tool required the generation of an experimental dataset that explores a diverse network of reactant pairings across a set of reaction conditions. A large scope of C–N couplings was actively learned by neural network models by using a systematic process to design experiments. The models showed good performance in experimental validation: Ten products were isolated in more than 85% yield from a range of couplings with out-of-sample reactants designed to challenge the models. Importantly, the developed workflow continually improves the prediction capability of the tool as the corpus of data grows.

Ring-opening polymerization of cyclic oligosiloxanes without producing cyclic oligomers

Limiao Shi, Aurélie Boulègue-Mondière, et. al

Abstract

A long-standing problem associated with silicone synthesis is contamination of the polymer products with 10 to 15% cyclic oligosiloxanes that results from backbiting reactions at the polymer chain ends. This process, in competition with chain propagation through ring-opening polymerization (ROP) of cyclic monomers, was thought to be unavoidable and routinely leads to a thermodynamically controlled reaction mixture (polymer/cyclic oligosiloxanes = 85/15). Here, we report that simple alcohol coordination to the anionic chain ends prevents the backbiting process and that a well-designed phosphonium cation acts as a self-quenching system in response to loss of coordinating alcohols to stop the reaction before the backbiting process begins. The combination of both effects allows a thermodynamically controlled ROP of the eight-membered siloxane ring D_4 without producing undesirable cyclic oligosiloxanes.

A microscale soft ionic power source modulates neuronal network activity

Zhang, Yujia, et. al

Abstract

Bio-integrated devices need power sources to operate[1,2]. Despite widely used technologies that can provide power to large-scale targets, such as wired energy supplies from batteries or wireless energy transduction[3], a need to efficiently stimulate cells and tissues on the microscale is still pressing. The ideal miniaturized power source should be biocompatible, mechanically flexible and able to generate an ionic current

for biological stimulation, instead of using electron flow as in conventional electronic devices[4,5,6]. One approach is to use soft power sources inspired by the electrical eel[7,8]; however, power sources that combine the required capabilities have not yet been produced, because it is challenging to obtain miniaturized units that both conserve contained energy before usage and are easily triggered to produce an energy output. Here we develop a miniaturized soft power source by depositing lipid-supported networks of nanolitre hydrogel droplets that use internal ion gradients to generate energy. Compared to the original eel-inspired design[7], our approach can shrink the volume of a power unit by more than 10^5-fold and it can store energy for longer than 24 h, enabling operation on-demand with a 680-fold greater power density of about 1,300 W m^{-3}. Our droplet device can serve as a biocompatible and biological ionic current source to modulate neuronal network activity in three-dimensional neural microtissues and in ex vivo mouse brain slices. Ultimately, our soft microscale ionotronic device might be integrated into living organisms.

BIOLOGY

An mTRAN-mRNA interaction mediates mitochondrial translation initiation in plants

Huy Cuong Tran, Vivian Schmitt, et al.

Abstract

Plant mitochondria represent the largest group of respiring organelles on the planet. Plant mitochondrial messenger RNAs (mRNAs) lack Shine-Dalgarno-like ribosome-binding sites, so it is unknown how plant mitoribosomes recognize mRNA. We show that "mitochondrial translation factors" mTRAN1 and mTRAN2 are land plant–specific proteins, required for normal mitochondrial respiration chain biogenesis. Our studies suggest that mTRANs are noncanonical pentatricopeptide repeat (PPR)–like RNA binding proteins of the mitoribosomal "small" subunit. We identified conserved Adenosine (A)/Uridine (U)-rich motifs in the 5′ regions of plant mitochondrial mRNAs. mTRAN1 binds this motif, suggesting that it is a mitoribosome homing factor to identify mRNAs. We demonstrate that mTRANs are likely required for translation of all plant mitochondrial mRNAs. Plant mitochondrial translation initiation thus appears to use a protein-mRNA interaction that is divergent from bacteria or mammalian mitochondria.

Editor: Chaoyi Chu（褚朝奕） TEL: 3548 Email: ccy@jsut.edu.cn

Genomic inference of a severe human bottleneck during the Early to Middle Pleistocene transition

Wangjie Hu, Ziqian Hao, et. al

Abstract

Population size history is essential for studying human evolution. However, ancient population size history during the Pleistocene is notoriously difficult to unravel. In this study, we developed a fast infinitesimal time coalescent process (FitCoal) to circumvent this difficulty and calculated the composite likelihood for present-day human genomic sequences of 3154 individuals. Results showed that human ancestors went through a severe population bottleneck with about 1280 breeding individuals between around 930,000 and 813,000 years ago. The bottleneck lasted for about 117,000 years and brought human ancestors close to extinction. This bottleneck is congruent with a substantial chronological gap in the available African and Eurasian fossil record. Our results provide new insights into our ancestry and suggest a coincident speciation event.

Cell polarity linked to gravity sensing is generated by LZY translocation from statoliths to the plasma membrane

Takeshi Nishimura, Shogo Mori, et. al

Abstract

Organisms have evolved under gravitational force, and many sense the direction of gravity by means of statoliths in specialized cells. In flowering plants, starch-accumulating plastids, known as amyloplasts, act as statoliths to facilitate downstream gravitropism. The gravity-sensing mechanism has long been considered a mechanosensing process by which amyloplasts transmit forces to intracellular structures, but the molecular mechanism underlying this has not been elucidated. We show here that LAZY1-LIKE (LZY) family proteins involved in statocyte gravity signaling associate with amyloplasts and the proximal plasma membrane. This results in polar localization according to the direction of gravity. We propose a gravity-sensing mechanism by which LZY translocation to the plasma membrane signals the direction of gravity by transmitting information on the position of amyloplasts.

Editor: Chaoyi Chu（褚朝奕） TEL: 3548 Email: ccy@jsut.edu.cn

Ⅲ Calling for papers

AI 2023

Submission deadline:	**Sep 16, 2023**
Conference date:	**Oct 21, 2023 - Oct 22, 2023**
Full name:	**International Conference on Artificial Intelligence and Applications**
Location:	**Sydney, Australia**
Website:	https://csty2023.org/ai/index

9th International Conference on Artificial Intelligence and Applications (AI 2023) will provide an excellent international forum for sharing knowledge and results in theory, methodology and applications of Artificial Intelligence and its applications. The Conference looks for significant contributions to all major fields of the Artificial Intelligence, Soft Computing in theoretical and practical aspects. The aim of the Conference is to provide a platform to the researchers and practitioners from both academia as well as industry to meet and share cutting-edge development in the field.

Authors are solicited to contribute to the conference by submitting articles that illustrate research results, projects, surveying works and industrial experiences that describe significant advances in the following areas, but are not limited to.

Call for papers:

AI Algorithms
Artificial Intelligence Tools and Application
Automatic Control
Bioinformatics
CAD Design and Testing
Computational Theories of Learning
Computer Vision and Speech Understanding
Data Mining and Machine Learning Tools
Fuzzy Logic
Heuristic and AI Planning Strategies and Tools
Hybrid Intelligent Systems
Information Retrieval
Intelligent System Architecture
Knowledge Representation
Natural Language Processing
Knowledge-based Systems
Mechatronics
Multimedia & Cognitive Informatics
Neural Networks
Parallel Processing
Pattern Recognition
Pervasive Computing and Ambient Intelligence
Programming Languages
Reasoning and Evolution
Recent Trends and Developments
Robotics
Semantic Web Techniques and Technologies
Soft computing theory and Applications
Software & Hardware Architectures
Web Intelligence Applications & Search

Editor: Chaoyi Chu（褚朝奕） TEL: 3548 Email: ccy@jsut.edu.cn

CGIP 2024

Submission deadline:	**Nov 20, 2022**
Conference date:	**Jan 12, 2024 - Jan 15, 2024**
Full name:	**International Conference on Computer Graphics and Image Processing**
Location:	**Kyoto, Japan**
Website:	http://www.cgip.org/

2024 2nd International Conference on Computer Graphics and Image Processing (CGIP 2024) which is sponsored by Tokai University and supported by Gifu University will be held during January 12-15, 2024 in Kyoto, Japan.

CGIP 2024 can provide opportunities for delegates to exchange new ideas and application experiences face to face, to establish business or research relations as well as to find global partners for future collaboration. For more conference information, please visit the conference website: http://www.cgip.org/.

Topics of Interest :

Computer Graphics and Photography Technology
Graphics Hardware
Graphical Human Computer Interfaces
Graphics System Architecture
Graphic Toolkits
Simulation for Computer Graphics
Shape and Image Retrieval
Parallel Graphics
GPU Graphics
Computational Photography
Multimedia and Web Graphics
Computer Vision and Image Processing
Computer Graphics
Image Processing
Image Based Rendering
Computer Vision
Visual Analytics
Pattern Recognition
Rendering and Animation
Rendering Techniques
Computer Animation
Sketch-Based Modeling

Editor: Chaoyi Chu（褚朝奕） TEL: 3548 Email: ccy@jsut.edu.cn

IEEE CAIT 2023

Submission deadline: **Sep 20, 2023**
Conference date: **Dec 13, 2023 - Dec 15, 2023**
Full name: **International Conference on Computers and Artificial Intelligence Technology**
Location: **Macau, China**
Website: http://www.cait.net/

IEEE 2023 4th International Conference on Artificial Intelligence Technology (CAIT 2023-www.cait.net) will be held during the period December 13-15, 2023 in Macau, China. The conference is sponsored by Macau University of Science and Technology, IEEE Macau, patrons with Beijing University of Posts and Telecommunications, Beijing Information Science and Technology University, Guangxi University, etc. CAIT focuses on the synergetic interaction of Artificial Intelligence Technology, and provide an excellent platform to all researchers share latest ideas. The mutual benefit make it possible to build and evolve new robotic systems, to reduce the development cost, and to enhance the quality.

Call for Papers:
Data Mining
Deep Learning
Computer vision
Pattern recognition
Artificial Neural Networks
Natural language processing
Robotics and intelligent systems
...
More topics, please visit: http://cait.net/cfp.html

DMDB 2024

Submission deadline: **Sep 23, 2023**
Conference date: **Jan 20, 2024 - Jan 21, 2024**
Full name: **International Conference on Data Mining and Database**
Location: **Zurich, Switzerland**
Website: https://ccseit2024.org/dmdb/index

11th International Conference on Data Mining and Database (DMDB 2024)provides a forum for researchers who address this issue and to present their work in a peer-reviewed forum. Authors are solicited to contribute to the conference by submitting articles that illustrate research results,

projects, surveying works and industrial experiences that describe significant advances in the following areas, but are not limited to these topics only.

***Call for papers:**

Data Mining

Data Mining Foundations
Data Mining Applications
Knowledge Processing

Data Base

Constraint Modeling and Processing
Data and Information Integration & Modeling
Data and Information Privacy and Security
Data and Information Quality
Data and Information Networks
Data and Information Semantics
Data and Information Streams
Data Management in Grid and P2P Systems
Data Mining Algorithms
Data Mining Systems, Data Warehousing, OLAP
Database and Information System Architecture and Performance
Data Structures and Data Management Algorithms
DB Systems & Applications
Digital Libraries
Distributed, Parallel, P2P and Grid-based Databases
Electronic Commerce and Web Technologies
Electronic Government & E-Participation
Expert Systems and Decision Support Systems
Expert Systems, Decision Support Systems & Applications
Information Retrieval and Database Systems
Information Systems
Interoperability
Knowledge Acquisition, Discovery & Management
Knowledge and Information Processing
Knowledge Modeling
Knowledge Processing
Metadata Management
Mobile Data and Information
Multi-Databases and Database Federation
Multimedia, Object, Object Relational and Deductive Databases
Pervasive Data and Information
Process Modeling
Process Support and Automation
Query Processing and Optimization
Semantic Web and Ontologies
Sensor Data Management
Statistical and Scientific Databases
Temporal, Spatial and High Dimensional Databases
Trust, Privacy & Security in Digital Business
User Interfaces to Databases and Information Systems
Very Large Data Bases
Workflow Management and Databases
WWW and Databases
XML and Databases

Editor: Chaoyi Chu（褚朝奕） TEL: 3548 Email: ccy@jsut.edu.cn

CACEE 2023

Submission deadline: **Sep 30, 2023**
Conference date: **Oct 20, 2023 - Oct 22, 2023**
Full name: **International Conference on Automation, Control and Electronics Engineering**
Location: **Chongqing, China**
Website: http://www.cacee2023.net/

2023 International Conference on Automation, Control and Electronics Engineering (CACEE 2023) will be held in Chongqing, China during October 20-22, 2023. CACEE is an annual conference which explores the development and implications in the related fields of Automation, Control and Electronics Engineering an objective to present the novel and fundamental advancements. It also serves to foster communication among researchers and practitioners working in a wide variety of scientific areas with a common interest in improving Automation, Control and Electronics Engineering. Featured with invited speeches and paper presentations, CACEE 2023 sincerely welcome interested researchers and professors to understand the frontier research trends and share latest research results, summarize current work and inspire scientific research ideas, broaden horizons and cultivate scientific research interest.

Topics of interest

Automated Guided Vehicles
Factory Modeling and Automation
Fault Detection
Manufacturing Control and Automation Engineering
Fuzzy and Neural Systems
Process Automation
Industrial Process Control
Sensor Networks and Networked Control
Intelligent and AI Based Control
Intelligent Automation
Man-machine Interactions
Process Control & Instrumentation
Material Processing and Control
Instruments and Vibration Control
Control Theory and Application
(For more topics: http://www.cacee2023.net/CFP.html)

Editor: Chaoyi Chu（褚朝奕） TEL: 3548 Email: ccy@jsut.edu.cn