Science Newsletter

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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 post several papers which are related to the top concerned topics of researches on Computer Science. The papers are classified in 5 categories, and they are: **Machine learning, Pattern recognition, Large language models, Big Data** and **Genetic Algorithm**. Also, the listed papers are all arranged in a descending sort of JCR impact factor. If you want full pages of these papers, please contact us for help.

MACHINE LEARNING

J Am Chem Soc (impact factor: 15) 1 区 TOP

Incorporating Synthetic Accessibility in Drug Design: Predicting Reaction Yields of Suzuki Cross-Couplings by Leveraging AbbVie's 15-Year Parallel Library Data Set.

Raghavan, Rago, et. al

Abstract:
Despite the increased use of computational tools to supplement medicinal chemists' expertise and intuition in drug design, predicting synthetic yields in medicinal chemistry endeavors remains an unsolved challenge. Existing design workflows could profoundly benefit from reaction yield prediction, as precious material waste could be

reduced, and a greater number of relevant compounds could be delivered to advance the design, make, test, analyze (DMTA) cycle. In this work, we detail the evaluation of AbbVie's medicinal chemistry library data set to build machine learning models for the prediction of Suzuki coupling reaction yields. The combination of density functional theory (DFT)-derived features and Morgan fingerprints was identified to perform better than one-hot encoded baseline modeling, furnishing encouraging results. Overall, we observe modest generalization to unseen reactant structures within the 15-year retrospective library data set. Additionally, we compare predictions made by the model to those made by expert medicinal chemists, finding that the model can often predict both reaction success and reaction yields with greater accuracy. Finally, we demonstrate the application of this approach to suggest structurally and electronically similar building blocks to replace those predicted or observed to be unsuccessful prior to or after synthesis, respectively. The yield prediction model was used to select similar monomers predicted to have higher yields, resulting in greater synthesis efficiency of relevant drug-like molecules.

Sci Total Environ (impact factor: 9.8) 1 区 TOP

Identifying interactive effects of spatial drivers in soil heavy metal pollutants using interpretable machine learning models.

Duan, Wang, et. al

Abstract:

The accurate identification of spatial drivers is crucial for effectively managing soil heavy metals (SHM). However, understanding the complex and diverse spatial drivers of SHM and their interactive effects remains a significant challenge. In this study, we present a comprehensive analysis framework that integrates Geodetector, CatBoost, and SHapley Additive exPlanations (SHAP) techniques to identify and elucidate the interactive effects of spatial drivers in SHM within the Pearl River Delta (PRD) region of China. Our investigation incorporated fourteen environmental factors and focused on the pollution levels of three prominent heavy metals: Hg, Cd, and Zn. These findings provide several key insights: (1) The distribution of SHM is influenced by the combined effects of various individual factors and interactions within the source-flow-sink process. (2) Compared with the spatial interpretation of individual factors, the interaction between Hg and Cd exhibited enhanced spatial explanatory power. Similarly, interactions involving Zn mainly demonstrated increased spatial explanatory power, but there was one exception in which a weakening was observed. (3) Spatial heterogeneity plays a crucial role in determining the contributions of environmental factors to soil heavy metal concentrations. Although individual factors generally promote metal accumulation, their effects fluctuate when interactions are considered. (4) The SHAP interpretable method effectively addresses the limitations associated with machine-learning models by providing understandable insights into heavy metal pollution. This enables a comparison of the importance of environmental factors and elucidates their directional impacts, thereby aiding in the understanding of interaction

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

mechanisms. The methods and findings presented in this study offer valuable insights into the spatial heterogeneity of heavy metal pollution in soil. By focusing on the effects of interactive factors, we aimed to develop more accurate strategies for managing SHM pollution.

Chest (impact factor: 9.6) 1 区 TOP

Differential Effect of PEEP Strategies in ARDS Patients: A Bayesian Analysis of Clinical Subphenotypes.

Siuba, Bulgarelli, et. al

Abstract:

Acute respiratory distress syndrome (ARDS) is a heterogeneous condition with two subphenotypes identified by different methodologies. Our group similarly identified two ARDS subphenotypes using nine routinely available clinical variables. However, whether these are associated with differential response to treatment has yet to be explored.Are there differential responses to positive end-expiratory pressure (PEEP) strategies on 28-day mortality according to subphenotypes in adult patients with ARDS?We evaluated data from two prior ARDS trials (ALVEOLI and ART) that compared different PEEP strategies. We classified patients into one of two subphenotypes as previously described. We assessed the differential effect of PEEP with a Bayesian hierarchical logistic model for the primary outcome of 28-day mortality.We analyzed data from 1559 ARDS patients. Compared to lower PEEP, a higher PEEP strategy resulted in higher 28-day mortality in subphenotype A patients in ALVEOLI (OR, 1.61 [95% CrI 0.90 to 2.94]) and ART (OR 1.73 [95% CrI 1.01 to 2.98]), with a probability of harm from higher PEEP in this subphenotype of 94.3% and 97.7% in ALVEOLI and ART, respectively. Higher PEEP was not associated with mortality in subphenotype B patients in each trial (OR, 0.95 [95% CrI, 0.51 to 1.73]) and (OR, 1.00 [95% CrI 0.63 to 1.55]); probability of benefit of 56.4% and 50.7% in ALVEOLI and ART, respectively. These effects were not modified by PaO2/FiO2 ratio, driving pressure, or the severity of illness for the cohorts.We found evidence of differential response to PEEP strategies across two ARDS subphenotypes, suggesting possible harm with a higher PEEP strategy in one subphenotype. These observations may assist with predictive enrichment in future clinical trials.Copyright © 2024. Published by Elsevier Inc.

PATTERN RECOGNITION

ACS Nano (impact factor: 17.1) 1 区 TOP

Programmable Retention Characteristics in MoS2-Based Atomristors for Neuromorphic and Reservoir Computing Systems.

Lee, Huang, et. al

Abstract:

In this study, we investigate the coexistence of short- and long-term memory effects owing to the programmable retention characteristics of a two-dimensional Au/MoS2/Au atomristor device and determine the impact of these effects on synaptic properties. This device is constructed using bilayer MoS2 in a crossbar structure. The presence of both short- and long-term memory characteristics is proposed by using a filament model within the bilayer transition-metal dichalcogenide. Short- and long-term properties are validated based on programmable multilevel retention tests. Moreover, we confirm various synaptic characteristics of the device, demonstrating its potential use as a synaptic device in a neuromorphic system. Excitatory postsynaptic current, paired-pulse facilitation, spike-rate-dependent plasticity, and spike-number-dependent plasticity synaptic applications are implemented by operating the device at a low-conductance level. Furthermore, long-term potentiation and depression exhibit symmetrical properties at high-conductance levels. Synaptic learning and forgetting characteristics are emulated using programmable retention properties and composite synaptic plasticity. The learning process of artificial neural networks is used to achieve high pattern recognition accuracy, thereby demonstrating the suitability of the use of the device in a neuromorphic system. Finally, the device is used as a physical reservoir with time-dependent inputs to realize reservoir computing by using short-term memory properties. Our study reveals that the proposed device can be applied in artificial intelligence-based computing applications by utilizing its programmable retention properties.

Nat Commun (impact factor: 16.6) 1 区

Medical history predicts phenome-wide disease onset and enables the rapid response to emerging health threats

Jakob Steinfeldt, Benjamin Wild, et al

Abstract:

The COVID-19 pandemic exposed a global deficiency of systematic, data-driven guidance to identify high-risk individuals. Here, we illustrate the utility of routinely recorded medical history to predict the risk for 1883 diseases across clinical specialties and support the rapid response to emerging health threats such as COVID-19. We developed a neural network to learn from health records of 502,460 UK Biobank. Importantly, we observed discriminative improvements over basic demographic

predictors for 1774 (94.3%) endpoints. After transferring the unmodified risk models to the All of US cohort, we replicated these improvements for 1347 (89.8%) of 1500 investigated endpoints, demonstrating generalizability across healthcare systems and historically underrepresented groups. Ultimately, we showed how this approach could have been used to identify individuals vulnerable to severe COVID-19. Our study demonstrates the potential of medical history to support guidance for emerging pandemics by systematically estimating risk for thousands of diseases at once at minimal cost.

Food Res Int (impact factor: 8.1) 1 ☒

The formation and conversion of characteristic aroma profiles and key harmful substances in different high-temperature processing of hairtail (Trichiurus Haumela).

Fu, Wang, et. al

Abstract:

The balance regulation between characteristic aroma and hazards in high-temperature processed fish is a hot spot. This study was aimed to explore the interactive relationship between the nutritional value, microstructures, aroma, and harmful substances of hairtail under different frying methods including traditional frying (TF), air frying (AF), and vacuum frying (VF) via chemical pattern recognition. The results indicated that VF-prepared hairtail could form a crunchy mouthfeel and retain the highest content of protein (645.53 mg/g) and the lowest content of fat (242.03 mg/g). Vacuum frying reduced lipid oxidation in hairtail, resulting in the POV reaching 0.02 mg/g, significantly lower than that of TF (0.05 mg/g) and AF (0.21 mg/g), and TBARS reached 0.83 mg/g, significantly lower than that of AF (1.96 mg/g) ($P < 0.05$), respectively. Notable variations were observedin the aroma profileof hairtail preparedfrom different frying methods. Vacuum frying of hairtail resulted in higher levels of pyrazines and alcohols, whereas traditional frying and air frying were associated with the formation of aldehydes and ketones, respectively. Air frying was not a healthy way to cook hairtail which produced the highest concentration of harmful substances (up to 190.63 ng/g), significantly higher than VF (5.72 ng/g) and TF (52.78 ng/g) ($P < 0.05$), especially norharman (122.57 ng/g), significantly higher than VF (4.50 ng/g) and TF (32.63 ng/g) ($P < 0.05$). Norharman and acrylamide were the key harmful substances in hairtail treated with traditional frying. The vacuum frying method was an excellent alternative for deep-fried hairtail as a snack food with fewer harmful substances and a fine aroma, providing a theoretic guidance for preparing healthy hairtail food with high nutrition and superior sensory attraction.

LARGE LANGUAGE MODELS

Nat Hum Behav (impact factor: 29.9) 1 ☒

Testing theory of mind in large language models and humans

James W. A. Strachan, Dalila Albergo, et. al

Abstract:

At the core of what defines us as humans is the concept of theory of mind: the ability to track other people's mental states. The recent development of large language models (LLMs) such as ChatGPT has led to intense debate about the possibility that these models exhibit behaviour that is indistinguishable from human behaviour in theory of mind tasks. Here we compare human and LLM performance on a comprehensive battery of measurements that aim to measure different theory of mind abilities, from understanding false beliefs to interpreting indirect requests and recognizing irony and faux pas. We tested two families of LLMs (GPT and LLaMA2) repeatedly against these measures and compared their performance with those from a sample of 1,907 human participants. Across the battery of theory of mind tests, we found that GPT-4 models performed at, or even sometimes above, human levels at identifying indirect requests, false beliefs and misdirection, but struggled with detecting faux pas. Faux pas, however, was the only test where LLaMA2 outperformed humans. Follow-up manipulations of the belief likelihood revealed that the superiority of LLaMA2 was illusory, possibly reflecting a bias towards attributing ignorance. By contrast, the poor performance of GPT originated from a hyperconservative approach towards committing to conclusions rather than from a genuine failure of inference. These findings not only demonstrate that LLMs exhibit behaviour that is consistent with the outputs of mentalistic inference in humans but also highlight the importance of systematic testing to ensure a non-superficial comparison between human and artificial intelligences.

Small (impact factor: 13.3) 2 ☒ TOP

Text-to-Microstructure Generation Using Generative Deep Learning.

Zheng, Watanabe, et. al

Abstract:

Designing novel materials is greatly dependent on understanding the design principles, physical mechanisms, and modeling methods of material microstructures, requiring experienced designers with expertise and several rounds of trial and error. Although recent advances in deep generative networks have enabled the inverse design of material microstructures, most studies involve property-conditional generation and focus on a specific type of structure, resulting in limited generation diversity and poor human-computer interaction. In this study, a pioneering text-to-microstructure deep

generative network (Txt2Microstruct-Net) is proposed that enables the generation of 3D material microstructures directly from text prompts without additional optimization procedures. The Txt2Microstruct-Net model is trained on a large microstructure-caption paired dataset that is extensible using the algorithms provided. Moreover, the model is sufficiently flexible to generate different geometric representations, such as voxels and point clouds. The model's performance is also demonstrated in the inverse design of material microstructures and metamaterials. It has promising potential for interactive microstructure design when associated with large language models and could be a user-friendly tool for material design and discovery.

J Am Med Inform Assoc (impact factor: 6.4) 2 ☒

Evaluating the accuracy of a state-of-the-art large language model for prediction of admissions from the emergency room.

Glicksberg, Timsina, et. al

Abstract:

Artificial intelligence (AI) and large language models (LLMs) can play a critical role in emergency room operations by augmenting decision-making about patient admission. However, there are no studies for LLMs using real-world data and scenarios, in comparison to and being informed by traditional supervised machine learning (ML) models. We evaluated the performance of GPT-4 for predicting patient admissions from emergency department (ED) visits. We compared performance to traditional ML models both naively and when informed by few-shot examples and/or numerical probabilities.We conducted a retrospective study using electronic health records across 7 NYC hospitals. We trained Bio-Clinical-BERT and XGBoost (XGB) models on unstructured and structured data, respectively, and created an ensemble model reflecting ML performance. We then assessed GPT-4 capabilities in many scenarios: through Zero-shot, Few-shot with and without retrieval-augmented generation (RAG), and with and without ML numerical probabilities.The Ensemble ML model achieved an area under the receiver operating characteristic curve (AUC) of 0.88, an area under the precision-recall curve (AUPRC) of 0.72 and an accuracy of 82.9%. The naïve GPT-4's performance (0.79 AUC, 0.48 AUPRC, and 77.5% accuracy) showed substantial improvement when given limited, relevant data to learn from (ie, RAG) and underlying ML probabilities (0.87 AUC, 0.71 AUPRC, and 83.1% accuracy). Interestingly, RAG alone boosted performance to near peak levels (0.82 AUC, 0.56 AUPRC, and 81.3% accuracy).The naïve LLM had limited performance but showed significant improvement in predicting ED admissions when supplemented with real-world examples to learn from, particularly through RAG, and/or numerical probabilities from traditional ML models. Its peak performance, although slightly lower than the pure ML model, is noteworthy given its potential for providing reasoning behind predictions. Further refinement of LLMs with real-world data is necessary for successful integration

BIG DATA

NPJ Digit Med (impact factor: 15.2) 1 区

Self-supervised learning of accelerometer data provides new insights for sleep and its association with mortality

Hang Yuan, Tatiana Plekhanova, et. al

Abstract

Sleep is essential to life. Accurate measurement and classification of sleep/wake and sleep stages is important in clinical studies for sleep disorder diagnoses and in the interpretation of data from consumer devices for monitoring physical and mental well-being. Existing non-polysomnography sleep classification techniques mainly rely on heuristic methods developed in relatively small cohorts. Thus, we aimed to establish the accuracy of wrist-worn accelerometers for sleep stage classification and subsequently describe the association between sleep duration and efficiency (proportion of total time asleep when in bed) with mortality outcomes. We developed a self-supervised deep neural network for sleep stage classification using concurrent laboratory-based polysomnography and accelerometry. After exclusion, 1448 participant nights of data were used for training. The difference between polysomnography and the model classifications on the external validation was 34.7 min (95% limits of agreement (LoA): −37.8–107.2 min) for total sleep duration, 2.6 min for REM duration (95% LoA: −68.4–73.4 min) and 32.1 min (95% LoA: −54.4–118.5 min) for NREM duration. The sleep classifier was deployed in the UK Biobank with 100,000 participants to study the association of sleep duration and sleep efficiency with all-cause mortality. Among 66,214 UK Biobank participants, 1642 mortality events were observed. Short sleepers (<6 h) had a higher risk of mortality compared to participants with normal sleep duration of 6–7.9 h, regardless of whether they had low sleep efficiency (Hazard ratios (HRs): 1.58; 95% confidence intervals (CIs): 1.19–2.11) or high sleep efficiency (HRs: 1.45; 95% CIs: 1.16–1.81). Deep-learning-based sleep classification using accelerometers has a fair to moderate agreement with polysomnography. Our findings suggest that having short overnight sleep confers mortality risk irrespective of sleep continuity.

Sci Total Environ (impact factor: 9.8) 1 ☒ TOP

Dissemination of antimicrobial resistance in agricultural ecosystems following irrigation with treated municipal wastewater.

Phan, Bhattacharjee, et. al

Abstract

The spread of antimicrobial resistance (AMR) in agricultural systems via irrigation water is a serious public health issue as it can be transmitted to humans through the food chain. Therefore, understanding the dissemination routes of antibiotic resistance genes (ARGs) in agricultural systems is crucial for the assessment of health risks associated with eating fresh vegetables such as spinach and radish irrigated with treated municipal wastewater (TMW). In this study, we investigated the bacterial community structure and resistome in the soil-plant-earthworm continuum after irrigation of spinach and radish with TMW containing the antibiotics trimethoprim (TMP), sulfamethoxazole (SMZ), and sulfapyridine (SPD) using 16S rRNA gene sequencing and high throughput quantitative PCR (HT-qPCR). The study was conducted in two phases: Phase I involved eight weeks of spinach and radish production using TMW for irrigation, whereas Phase II entailed three weeks of earthworm exposure to contaminated plant material obtained in Phase I. The 16S data indicated that the rhizosphere bacterial community composition and structure were more resilient to antibiotic residuals in the irrigated water, with radish showing less susceptibility than spinach than those of bulk soils. The HT-qPCR analysis revealed that a total of 271 ARGs (out of 285) and 9 mobile genetic elements (MGEs) (out of 10) were detected in all samples. Higher diversity and abundance of ARGs were observed for samples irrigated with higher concentrations of antibiotics in both spinach and radish treatments. However, compared to spinach, radish ARG dynamics in the soil biome were more stable due to the change of antibiotic introduction to the soil. At the class level, multi-drug resistance (MDR) class was altered significantly by the presence of antibiotics in irrigation water. Compared to earthworm fecal samples, their corresponding soil environments showed a higher number of detected ARGs, suggesting that earthworms could play a role in reducing ARG dissemination in the soil environments. These findings will not only provide insight into the dissemination of ARGs in agricultural environments due to antibiotic residuals in irrigated water but could help understand the potential human health risks associated with ARGs.

Int J Biol Macromol (impact factor: 8.2) 1 ☒

Exploration of novel trehalases from cold-adapted Variovorax sp. PAMC28711: Functional characterization.

Shrestha, Karmacharya i, et. al

Abstract

The cold-adapted bacterium Variovorax sp. PAMC28711 possesses two distinct glycoside hydrolase (GH) families of trehalase, GH15 and GH37. While numerous studies have explored bacterial trehalase, the presence of two different trehalase genes within a single strain has not been reported until now. Interestingly, despite both GH37 and GH15 trehalases serving the same purpose of degrading trehalose, but do not share the sequence similarity. The substrate specificity assay confirmed that Vtre37 and Vtre15 displayed hydrolytic activity on α, α-trehalose. The key catalytic sites were identified as D280 and E469 in Vtre37 and E389 and E554 in Vtre15 through site-directed mutation and confirmed these two enzymes belong to trehalase. In addition, Vtre37 exhibited a relatively high level of enzyme activity of 1306.33 (±53.091) μmolmg-1, whereas Vtre15 showed enzyme activity of 408.39 (±12.503) μmolmg-1. Moreover, Vtre37 performed admirably showing resistance to ethanol (10 %), with high stable at acidic pH range. Furthermore, both prediction and experimental results indicate that validoxylamine A showed a potent inhibitory activity against Vtre37 trehalase with a Ki value of 16.85 nM. Therefore, we postulate that Vtre37 could be utilized as an ethanol enhancer and designed for screening inhibitors related to the trehalose degradation pathway. Additionally, we believe that characterizing these bacterial trehalase contributes to a better understanding of trehalose metabolism and its biological importance in bacteria.Copyright © 2024. Published by Elsevier B.V.

GENETIC ALGORITHM

Nat Commun (impact factor: 16.6) 1 ☒

Development of a long noncoding RNA-based machine learning model to predict COVID-19 in-hospital mortality

Yvan Devaux, Lu Zhang, et. al

Abstract

Tools for predicting COVID-19 outcomes enable personalized healthcare, potentially easing the disease burden. This collaborative study by 15 institutions across Europe aimed to develop a machine learning model for predicting the risk of in-hospital mortality post-SARS-CoV-2 infection. Blood samples and clinical data from 1286 COVID-19 patients collected from 2020 to 2023 across four cohorts in Europe and Canada were analyzed, with 2906 long non-coding RNAs profiled using targeted sequencing. From a discovery cohort combining three European cohorts and 804 patients, age and the long non-coding RNA LEF1-AS1 were identified as predictive features, yielding an AUC of 0.83 (95% CI 0.82–0.84) and a balanced accuracy of 0.78 (95% CI 0.77–0.79) with a feedforward neural network classifier. Validation in an

independent Canadian cohort of 482 patients showed consistent performance. Cox regression analysis indicated that higher levels of LEF1-AS1 correlated with reduced mortality risk (age-adjusted hazard ratio 0.54, 95% CI 0.40–0.74). Quantitative PCR validated LEF1-AS1's adaptability to be measured in hospital settings. Here, we demonstrate a promising predictive model for enhancing COVID-19 patient management.

Cell Biol Toxicol (impact factor: 6.1) 2 区

Spatial transcriptomics reveals gene interactions and signaling pathway dynamics in rat embryos with anorectal malformation

Chen-Yi Wang, Mu-Yu Li, et. al

Abstract:

Anorectal malformation (ARM) is a prevalent early pregnancy digestive tract anomaly. The intricate anatomy of the embryonic cloaca region makes it challenging for traditional high-throughput sequencing methods to capture location-specific information. Spatial transcriptomics was used to sequence libraries of frozen sections from embryonic rats at gestational days (GD) 14 to 16, covering both normal and ARM cases. Bioinformatics analyses and predictions were performed using methods such as WGCNA, GSEA, and PROGENy. Immunofluorescence staining was used to verify gene expression levels. Gene expression data was obtained with anatomical annotations of clusters, focusing on the cloaca region's location-specific traits. WGCNA revealed gene modules linked to normal and ARM cloacal anatomy development, with cooperation between modules on GD14 and GD15. Differential gene expression profiles and functional enrichment were presented. Notably, protein levels of Pcsk9, Hmgb2, and Sod1 were found to be downregulated in the GD15 ARM hindgut. The PROGENy algorithm predicted the activity and interplay of common signaling pathways in embryonic sections, highlighting their synergistic and complementary effects. A competing endogenous RNA (ceRNA) regulatory network was constructed from whole transcriptome data. Spatial transcriptomics provided location-specific cloaca region gene expression. Diverse bioinformatics analyses deepened our understanding of ARM's molecular interactions, guiding future research and providing insights into gene regulation in ARM development.

Med Sci Sports Exerc (impact factor: 4.1) 2 区 TOP

Self-Supervised Machine Learning to Characterise Step Counts from Wrist-Worn Accelerometers in the UK Biobank.

Small, Chan, et. al

Abstract:

Step count is an intuitive measure of physical activity frequently quantified in health-

related studies; however, accurate step counting is difficult in the free-living environment, with error routinely above 20% in wrist-worn devices against camera-annotated ground truth. This study aims to describe the development and validation of step count derived from a wrist-worn accelerometer and assess its association with cardiovascular and all-cause mortality in a large prospective cohort.We developed and externally validated a self-supervised machine learning step detection model, trained on an open-source and step-annotated free-living dataset. 39 individuals will free-living ground-truth annotated step counts were used for model development. An open-source dataset with 30 individuals was used for external validation. Epidemiological analysis was performed using 75,263 UK Biobank participants without prevalent cardiovascular disease (CVD) or cancer. Cox regression was used to test the association of daily step count with fatal CVD and all-cause mortality after adjustment for potential confounders.The algorithm substantially outperformed reference models (free-living mean absolute percent error of 12.5%, versus 65-231%). Our data indicate an inverse dose-response association, where taking 6,430-8,277 daily steps was associated with 37% [25-48%] and 28% [20-35%] lower risk of fatal CVD and all-cause mortality up to seven years later, compared to those taking fewer steps each day.We have developed an open and transparent method that markedly improves the measurement of steps in large-scale wrist-worn accelerometer datasets. The application of this method demonstrated expected associations with CVD and all-cause mortality, indicating excellent face validity. This reinforces public health messaging for increasing physical activity and can help lay the groundwork for the inclusion of target step counts in future public health guidelines.

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

Ⅱ Concentration

PHYSICS

Coexistence of superconductivity with partially filled stripes in the Hubbard model

Hao Xu, Chia-Min Chung, et al.

Abstract

The Hubbard model is an iconic model in quantum many-body physics and has been intensely studied, especially since the discovery of high-temperature cuprate superconductors. Combining the complementary capabilities of two computational methods, we found superconductivity in both the electron- and hole-doped regimes of the two-dimensional Hubbard model with next-nearest-neighbor hopping. In the electron-doped regime, superconductivity was weaker and was accompanied by antiferromagnetic Néel correlations at low doping. The strong superconductivity on the hole-doped side coexisted with stripe order, which persisted into the overdoped region with weaker hole-density modulation. These stripe orders varied in fillings between 0.6 and 0.8. Our results suggest the applicability of the Hubbard model with next-nearest hopping for describing cuprate high–transition temperature (T_c) superconductivity.

An atomic boson sampler

Aaron W. Young, Shawn Geller, et al.

Abstract

A boson sampler implements a restricted model of quantum computing. It is defined by the ability to sample from the distribution resulting from the interference of identical bosons propagating according to programmable, non-interacting dynamics[1]. An efficient exact classical simulation of boson sampling is not believed to exist, which has motivated ground-breaking boson sampling experiments in photonics with increasingly many photons[2,3,4,5,6,7,8,9,10,11,12]. However, it is difficult to generate and reliably evolve specific numbers of photons with low loss, and thus probabilistic techniques for postselection[7] or marked changes to standard boson sampling[10,11,12] are generally used. Here, we address the above challenges by implementing boson sampling using ultracold atoms[13,14] in a two-dimensional, tunnel-coupled optical lattice. This demonstration is enabled by a previously unrealized combination of tools involving high-fidelity optical cooling and imaging of atoms in a lattice, as well as programmable control of those atoms using optical tweezers. When extended to

interacting systems, our work demonstrates the core abilities required to directly assemble ground and excited states in simulations of various Hubbard models[15,16].

Observation of Nagaoka polarons in a Fermi–Hubbard quantum simulator

Martin Lebrat, Muqing Xu, et al.

Abstract

Quantum interference can deeply alter the nature of many-body phases of matter[1]. In the case of the Hubbard model, Nagaoka proved that introducing a single itinerant charge can transform a paramagnetic insulator into a ferromagnet through path interference[2,3,4]. However, a microscopic observation of this kinetic magnetism induced by individually imaged dopants has been so far elusive. Here we demonstrate the emergence of Nagaoka polarons in a Hubbard system realized with strongly interacting fermions in a triangular optical lattice[5,6]. Using quantum gas microscopy, we image these polarons as extended ferromagnetic bubbles around particle dopants arising from the local interplay of coherent dopant motion and spin exchange. By contrast, kinetic frustration due to the triangular geometry promotes antiferromagnetic polarons around hole dopants[7]. Our work augurs the exploration of exotic quantum phases driven by charge motion in strongly correlated systems and over sizes that are challenging for numerical simulation[8,9,10].

MATERIALS

Catalog of topological phonon materials

Yuanfeng Xu, M. G. Vergniory, et al.

Abstract

Phonons play a crucial role in many properties of solid-state systems, and it is expected that topological phonons may lead to rich and unconventional physics. On the basis of the existing phonon materials databases, we have compiled a catalog of topological phonon bands for more than 10,000 three-dimensional crystalline materials. Using topological quantum chemistry, we calculated the band representations, compatibility relations, and band topologies of each isolated set of phonon bands for the materials in the phonon databases. Additionally, we calculated the real-space invariants for all the topologically trivial bands and classified them as atomic or obstructed atomic bands. We have selected more than 1000 “ideal” nontrivial phonon materials to motivate future experiments. The datasets were used to build the Topological Phonon Database.

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

Large quantum anomalous Hall effect in spin-orbit proximitized rhombohedral graphene

Tonghang Han, Zhengguang Lu, et al.

Abstract

The quantum anomalous Hall effect (QAHE) is a robust topological phenomenon that features quantized Hall resistance at zero magnetic field. We report the QAHE in a rhombohedral pentalayer graphene-monolayer tungsten disulfide (WS_2) heterostructure. Distinct from other experimentally confirmed QAHE systems, this system has neither magnetic element nor moiré superlattice effect. The QAH states emerge at charge neutrality and feature Chern numbers $C = \pm 5$ at temperatures of up to about 1.5 kelvin. This large QAHE arises from the synergy of the electron correlation in intrinsic flat bands of pentalayer graphene, the gate-tuning effect, and the proximity-induced Ising spin-orbit coupling. Our experiment demonstrates the potential of crystalline two-dimensional materials for intertwined electron correlation and band topology physics and may enable a route for engineering chiral Majorana edge states.

Growth of diamond in liquid metal at 1 atm pressure

Gong, Yan, Luo, et al.

Abstract

Natural diamonds were (and are) formed (thousands of million years ago) in the upper mantle of Earth in metallic melts at temperatures of 900–1,400 °C and at pressures of 5–6 GPa (refs. [1,2]). Diamond is thermodynamically stable under high-pressure and high-temperature conditions as per the phase diagram of carbon[3]. Scientists at General Electric invented and used a high-pressure and high-temperature apparatus in 1955 to synthesize diamonds by using molten iron sulfide at about 7 GPa and 1,600 °C (refs. [4,5,6]). There is an existing model that diamond can be grown using liquid metals only at both high pressure and high temperature[7]. Here we describe the growth of diamond crystals and polycrystalline diamond films with no seed particles using liquid metal but at 1 atm pressure and at 1,025 °C, breaking this pattern. Diamond grew in the subsurface of liquid metal composed of gallium, iron, nickel and silicon, by catalytic activation of methane and diffusion of carbon atoms into and within the subsurface regions. We found that the supersaturation of carbon in the liquid metal subsurface leads to the nucleation and growth of diamonds, with Si playing an important part in stabilizing tetravalently bonded carbon clusters that play a part in nucleation. Growth of (metastable) diamond in liquid metal at moderate temperature and 1 atm pressure opens many possibilities for further basic science studies and for the scaling of this type of growth.

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

CHEMISTRY

The odd-number cyclo[13]carbon and its dimer, cyclo[26]carbon

Florian Albrecht, Igor Rončević, et. al

Abstract

Molecular rings of *N* carbon atoms (cyclo[*N*]carbons, or C_N) are excellent benchmarking systems for testing quantum chemical theoretical methods and valuable precursors to other carbon-rich materials. Odd-*N* cyclocarbons, which have been elusive to date, are predicted to be even less stable than even-*N* cyclocarbons. We report the on-surface synthesis of cyclo[13]carbon, C_{13}, by manipulation of decachlorofluorene with a scanning probe microscope tip. We elucidated the properties of C_{13} by experiment and theoretical modeling. C_{13} adopts an open-shell configuration with a triplet ground state and a kinked geometry, which shows different extents of distortion and carbene localization depending on the molecular environment. Moreover, we prepared and characterized the C_{13} dimer, cyclo[26]carbon, demonstrating the potential of cyclocarbons and their precursors as building blocks for carbon allotropes.

Scalable decarboxylative trifluoromethylation by ion-shielding heterogeneous photoelectrocatalysis

Yixin Chen, Yuchen He, et. al

Abstract

Electrochemistry offers a sustainable synthesis route to value-added fine chemicals but is often constrained by competing electron transfer between the electrode and redox-sensitive functionalities distinct from the target site. Here, we describe an ion-shielding heterogeneous photoelectrocatalysis strategy to impose mass-transfer limitations that invert the thermodynamically determined order of electron transfer. This strategy is showcased to enable decarboxylative trifluoromethylation of sensitive (hetero)arenes by using trifluoroacetate, an inexpensive yet relatively inert trifluoromethyl group (CF_3) source. An ion-shielding layer, formed by trifluoroacetate anions electrostatically adsorbed on a positive molybdenum-doped tungsten trioxide (WO_3) photoanode, prevents undesired electron transfer between substrates and photogenerated holes. The practicality of the developed method was demonstrated with robust photoanode stability (approximately 380 hours), a good substrate scope, and scaling capability to achieve 100-gram synthesis by using photoelectrochemical flow cells.

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

Atomically dispersed hexavalent iridium oxide from MnO2 reduction for oxygen evolution catalysis

Ailong Li, Shuang Kong, et. al

Abstract

Hexavalent iridium (Ir^{VI}) oxide is predicted to be more active and stable than any other iridium oxide for the oxygen evolution reaction in acid; however, its experimental realization remains challenging. In this work, we report the synthesis, characterization, and application of atomically dispersed Ir^{VI} oxide (Ir^{VI}-*ado*) for proton exchange membrane (PEM) water electrolysis. The Ir^{VI}-*ado* was synthesized by oxidatively substituting the ligands of potassium hexachloroiridate(IV) (K_2IrCl_6) with manganese oxide (MnO_2). The mass-specific activity (1.7×10^5 amperes per gram of iridium) and turnover number (1.5×10^8) exceeded those of benchmark iridium oxides, and in situ x-ray analysis during PEM operations manifested the durability of Ir^{VI} at current densities up to 2.3 amperes per square centimeter. The high activity and stability of Ir^{VI}-*ado* showcase its promise as an anode material for PEM electrolysis.

BIOLOGY

A petavoxel fragment of human cerebral cortex reconstructed at nanoscale resolution

Alexander Shapson-Coe, Michał Januszewski, et al.

Abstract

To fully understand how the human brain works, knowledge of its structure at high resolution is needed. Presented here is a computationally intensive reconstruction of the ultrastructure of a cubic millimeter of human temporal cortex that was surgically removed to gain access to an underlying epileptic focus. It contains about 57,000 cells, about 230 millimeters of blood vessels, and about 150 million synapses and comprises 1.4 petabytes. Our analysis showed that glia outnumber neurons 2:1, oligodendrocytes were the most common cell, deep layer excitatory neurons could be classified on the basis of dendritic orientation, and among thousands of weak connections to each neuron, there exist rare powerful axonal inputs of up to 50 synapses. Further studies using this resource may bring valuable insights into the mysteries of the human brain.

Indian Ocean temperature anomalies predict long-term global dengue trends

Yuyang Chen, Yiting Xu, et. al

Abstract

Despite identifying El Niño events as a factor in dengue dynamics, predicting the oscillation of global dengue epidemics remains challenging. Here, we investigate climate indicators and worldwide dengue incidence from 1990 to 2019 using climate-driven mechanistic models. We identify a distinct indicator, the Indian Ocean basin-wide (IOBW) index, as representing the regional average of sea surface temperature anomalies in the tropical Indian Ocean. IOBW is closely associated with dengue epidemics for both the Northern and Southern hemispheres. The ability of IOBW to predict dengue incidence likely arises as a result of its effect on local temperature anomalies through teleconnections. These findings indicate that the IOBW index can potentially enhance the lead time for dengue forecasts, leading to better-planned and more impactful outbreak responses.

A nasal chemosensation–dependent critical window for somatosensory development

Linbi Ca, Ali Özgür Argunşah, et. al

Abstract

Nasal chemosensation is considered the evolutionarily oldest mammalian sense and, together with somatosensation, is crucial for neonatal well-being before auditory and visual pathways start engaging the brain. Using anatomical and functional approaches in mice, we reveal that odor-driven activity propagates to a large part of the cortex during the first postnatal week and enhances whisker-evoked activation of primary whisker somatosensory cortex (wS1). This effect disappears in adult animals, in line with the loss of excitatory connectivity from olfactory cortex to wS1. By performing neonatal odor deprivation, followed by electrophysiological and behavioral work in adult animals, we identify a key transient regulation of nasal chemosensory information necessary for the development of wS1 sensory-driven dynamics and somatosensation. Our work uncovers a cross-modal critical window for nasal chemosensation–dependent somatosensory functional maturation.

Ⅲ Calling for papers

SPTM 2024

Submission deadline:	**May 25, 2024**
Conference date:	**Jun 22, 2024 - Jun 23, 2024**
Full name:	**International Conference of Security, Privacy and Trust Management**
Location:	**Sydney, Australia**
Website:	https://csit2024.org/sptm/index

12th International Conference of Security, Privacy and Trust Management (SPTM 2024) looks for significant contributions to Trust management for networks. Original papers are invited on Security, Privacy and Trust Management of wireless and wired networks. The goal of this Conference is to bring together researchers and practitioners from academia and industry to focus on advanced networking concepts and establishing new collaborations in these areas.
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:
Trust, Security, Privacy, Policy management
Agent Based Trust Management
Authorization, Authentication and Identity Management
Pervasive Computation Trust
Cloud, P2P, Clusters and Grid Computing : Security and Role of Trust
Decentralized Trust Management
Trust in Service-Oriented Architecture- Open Architecture and Services
Social Networks & Web 2.0 Trust Management
Trust Management system for Wireless, Mobile and Sensor networks
Policy of Trust in E-leaning systems
Trust/risk based security frameworks
Trust Management for virtual organizations
Trust and Reputation Management
Multimedia Content Management

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

NCWMC 2024

Submission deadline:	**May 28, 2024**
Conference date:	**Sep 21, 2024 - Sep 22, 2024**
Full name:	**9th International Conference on Networks, Communications, Wireless and Mobile Computing**
Location:	**Copenhagen, Denmark**
Website:	https://ccsit2024.org/ncwmc/index

9th International Conference on Networks, Communications, Wireless and Mobile Computing (NCWMC 2024) looks for significant contributions to the Computer Networks, Communications, wireless and mobile computing for wired and wireless networks in theoretical and practical aspects. Original papers are invited on computer Networks, network protocols and wireless networks, Data communication Technologies, network security and mobile computing. The goal of this Conference is to bring together researchers and practitioners from academia and industry to focus on advanced networking concepts and establishing new collaborations in these areas.

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.

Topics of Interest :

Communication Network Architectures and Design
Communication Network Protocols
Discrete Algorithms and Discrete Modeling
Emerging Technologies for Next Generation Network
Future Internet Architecture, Protocols and Services
Mobile and Wireless Networks
Network Applications
Network Operation and Management
Network Security and Privacy
Network Services and Applications
Ubiquitous Networks and Cloud Computing
Wireless and Mobile Computing
Algorithms and Modeling for Tracking and Locating Mobile Users
Cryptography, Security and Privacy of mobile and Wireless Networks
Data Management on Mobile and Wireless Computing
Integration of Wired and Wireless Systems
Mobile Ad Hoc and Sensor networks
Performance of Mobile and Wireless Networks and Systems
Recent Trends in Mobile and Wireless Applications
Resource Management in mobile, Wireless and Ad-Hoc Networks
Routing, and Communication primitives in Ad Hoc and Sensor Networks
Satellite Communications
Service Creation and Management Environments for Mobile/Wireless Systems
Synchronization and Scheduling Issues in Mobile and Ad Hoc Networks
Wireless & Mobile Issues related to OS
Wireless Multimedia Systems

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

ACCC 2024

Submission deadline: **May 30, 2024**
Conference date: **Dec 20, 2024 - Dec 22, 2024**
Full name: **5th Asia Conference on Computers and Communications**
Location: **Shanghai, China**
Website: http://accc.net/

2024 The 5th Asia Conference on Computers and Communications (ACCC 2024) will be held in Singapore during December 20-22, 2024. ACCC is an annual conference since 2020, which aims to offer the communication for scholars to present the latest research and results of scientists, to create an opportunity to build networks with other academics and experts, to collect and publish academic papers with high quality,etc.

ACCC will gather the scholars from the world to discuss the hot topics in the field of computer and communications such as 5G, AI in Communication, Big Data, Blockchain Technology, Computer Architecture, Image Processing, Network Security and Cryptography, Virtual Reality and Visualization, Wireless and Sensor Devices, etc. ACCC features keynote and invited speeches as well as peer-reviewed paper presentations. And an optional social program is set up to offer more chance for interested scholars. The conference is completely open (one needs to register first), you will not have to be an author or a discussant to attend. On behalf of the Organizing Committee, we warmly invite you, computer and communications scientists, engineers or technicians,students, or simply interested by the technique, to take part in this unique and innovative conference with your enthusiasm to develop. Maybe your idea is still an idea, which hasn't been proved or accepted, but new ideas and innovation will be 100 percent respected in our conferences.

We are looking forward to meeting you in Singapore!

Call for Papers:

==Computer

► Algorithms
► Autonomic and Trusted Computing
►5G
► AI in Communication
► Artificial Intelligence and Machine Learning
► Big Data
► Blockchain Technology
► Biomedical Informatics and Computation
► Computer Architecture
► Data Compression
► High-Performance Computing
► Image Processing

==Communications

► RF and Microwave Communication
► Antenna and Propagation
► Microwave Theory and Techniques
► Remote Sensing and GPS
► Integrated Optics and Electro-optics Devices
► Techniques of Laser and Applications of Electro-optics
► Signal, Image and Video Processing
► Modulation, Coding, and Channel Analysis
► Electromagnetic and Photonics
► Optical Electronic Devices & Photonics

More topics, please visit: http://accc.net/topic.html

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

CECCC 2024

Submission deadline: **May 30, 2024**
Conference date: **Oct 18, 2024 - Oct 20, 2024**
Full name: **6th International Communication Engineering and Cloud Computing Conference**
Location: **Chengdu, China**
Website: http://www.ceccc.org/

The 2024 6th International Communication Engineering and Cloud Computing Conference (CECCC-2024) is scheduled to take place in Chengdu, China during October 18-20, 2024. CECCC2024 is mainly co-sponsored by Southwest Jiaotong University, Nanjing University of Science and Technology, and IEEE, also jointly supported by Sichuan University, Southwestern University of Finance and Economics, NOVA University of Lisbon, Portugal, etc. The primary objective of the conference is to bring together scientists, professors, research scholars, students, and industrial experts in the field of Communication and Computing to share innovative scientific information, promote national and international collaboration, and facilitate networking among universities and institutions. The conference aims to promote the transformation of fundamental research into institutional and industrialized research and convert applied exploration into real-time application, ultimately advancing the field of Communication Engineering and Cloud Computing.

***Call for papers:**

Track I: Communication
-Cognitive Radio and Cognitive Networks
-Communication Systems
-Future Internet and Next-Generation Networking Architectures
-High Performance Networks and Protocols
-Information Theory and Coding
-Internet measurement, modeling, and visualization
-Network Simulation and Emulation
-Optical Networks and Systems
-Satellite and Space Communications
-Sensor Networks and Embedded Systems
-Network Security
-Multimedia Networking

Track II: Computing
-Artificial Intelligence and Machine Learning
-Autonomic and Trusted Computing
-Big Data, Data Management and Analytics
-Cloud, Cluster, Grid and P2P Computing
-Computational Intelligence
-Computer Graphics, Simulation and Modeling
-Cryptography and Applied Mathematics
-Data Management, Exploration and Mining
-Natural Language Processing and Machine Translation
-Parallel and Distributed Algorithms
-Quantum Computing
-Signal and Image Processing
More Topics, please visit at http://www.ceccc.org/cfp.html

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ARAEML 2024

Submission deadline:	**May 30, 2024**
Conference date:	**Jun 28, 2024 - Jun 30, 2024**
Full name:	**International Conference on Advanced Robotics, Automation Engineering and Machine Learning**
Location:	**Hangzhou, China**
Website:	http://www.araeml.net/

2024 International Conference on Advanced Robotics, Automation Engineering and Machine Learning (ARAEML 2024), the conference will be held in Hangzhou, China during June 28-30, 2024. ARAEML 2024 is dedicated to addressing the challenges in the areas of Advanced Robotics, Automation Engineering and Machine Learning as well as its applications, presenting the latest scientific research results related to these topics. ARAEML 2024 looks forward to bringing together researchers and practitioners from academia and industries to focus on related topics and establishing new collaboration in these areas.

Topics of interest

Robot Control & Mobile Robotics
Mobile Sensor Networks
Robot Design, Development and Control
Perception and Awareness
Micro Robots and Micro-manipulation
Search, Rescue and Field Robotics
Robot Sensing and Data Fusion
Medical Robots and Bio-robotics & Human Centered Systems
Space and Underwater Robots
Cognitive Approach for Robotics & Mobile Robots
Visual Computing & Intelligent Robotics
Artificial Intelligence
Automated Guided Vehicles
Intelligent Automation
(For more topics: http://www.araeml.net/submission.html)

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