

Science Newsletter

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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/2025/0228/c5474a193334/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, Fuzzy control, Data Mining, IoT and Evolutionary computing**. 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

Brief Bioinform (impact factor: 7.7) 2 TOP

Advancing ADMET prediction through multiscale fragment-aware pretraining with MSformer-ADMET.

Huihui Liu, Bingjie Zhu, et. al

Abstract:

Absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties are critical determinants of the pharmacokinetic and safety profiles of drug candidates. Accurate and early-stage prediction of ADMET characteristics is essential for reducing

late-stage attrition rates, lowering development costs, and accelerating the drug discovery process. Recent advances in deep learning have shown great promise in molecular property prediction, especially with the emergence of Transformer-based architectures that can effectively model long-range dependencies in molecular representations. However, most existing methods rely heavily on atom-level encodings (e.g. smiles or molecular graphs), which often lack structural interpretability and generalization across heterogeneous tasks. Previously, we developed a de novo and flexible molecular representation framework named MSformer (available at <https://github.com/ZJUFanLab/MSformer>), which demonstrated success in bioactivity prediction. We have now adapted and specialized this architecture for ADMET property prediction. This adapted implementation, designated as MSformer-ADMET, extends the framework's capabilities to pharmacokinetic and toxicity endpoints while maintaining its flexible, fragmentation-based approach to molecular representation learning. MSformer-ADMET is fine-tuned on 22 tasks collected from the Therapeutics Data Commons (TDC), covering both classification and regression settings. Results demonstrate that MSformer-ADMET achieves superior performance across a wide range of ADMET endpoints, consistently outperforming conventional smiles-based and graph-based models. Notably, we further conducted interpretability analyses by leveraging the model's attention distributions and fragment-to-atom mappings, allowing the identification of key structural fragments that are highly associated with molecular properties. This post hoc interpretability provides more transparent insights into the structure-property relationship. Collectively, results demonstrate that MSformer-ADMET is a highly effective and broadly applicable model for ADMET prediction. © The Author(s) 2025. Published by Oxford University Press.

Nanoscale (impact factor: 5.1) 3  TOP

Device-level modelling for predicting the total density of states of single-walled CNTs with increasing chirality: a fusion of ab initio modeling and a machine learning framework.

Vusala Jafarova, Debarati Roy, et. al

Abstract:

The electronic properties of single-walled carbon nanotubes (SWCNTs) are highly sensitive to their chirality, influencing their potential applications in nanoelectronics and energy storage. This study presents a novel approach for predicting the distribution of the total density of states (TDOS) in SWCNTs as a function of chirality, integrating ab initio modeling with machine learning techniques. First-principles calculations based on density functional theory (DFT) are employed to establish a comprehensive dataset of TDOS values across various chiral indices. Machine learning models, trained on this dataset, are then utilized to generalize and predict trends in the electronic behavior of previously computed chirality configurations. The integration of computational physics with artificial intelligence enables a more efficient exploration of the electronic structure of SWCNTs, significantly reducing computational costs

while maintaining high predictive accuracy. The proposed framework enhances the understanding of chirality-dependent electronic properties and paves the way for the tailored design of carbon-based nanomaterials for advanced technological applications. In this study, we simulated the electronic properties of carbon nanotubes (CNTs) with chirality of (n,m) (here, $n = 4, 5, 6, \dots, 10$; $m = 0$). Our first-principles simulations predicted that SWCNT systems with ($n = 4, 5, 6$; $m = 0$) chirality have a metallic character. The metallicities of the (4,0), (5,0), and (6,0) systems are due to the strong σ^* - and π^* -mixing caused by the large curvature of the tube. In contrast, in the SWCNT ($n = 4, 5, 6$; $m = 0$) systems, the SWCNT compounds with ($n = 7, 8, 9, 10$; $m = 0$) chirality demonstrate semiconducting characteristics with narrow band gaps of 0.10-0.82 eV, and we conclude that these systems are direct band gap materials.

J Neurotrauma (impact factor: 3.8) 2 ☒

Intracranial Pressure as a Dynamic Predictor of Traumatic Brain Injury Outcomes: A Scoping Review.

John Kanter, Robert Osorio, Liu, et. al

Abstract:

Intracranial pressure (ICP) monitoring remains a cornerstone in the management of severe traumatic brain injury (TBI), yet its utility as a dynamic predictor of outcomes continues to evolve. We aimed to examine the role of serial ICP measurements as a potential predictor of outcomes after TBI, to combine ICP data with cerebrovascular reactivity metrics, and to highlight emerging trends in ICP modeling such as machine learning-based predictive models. We conducted a rigorous scoping review following Preferred Reporting Items for Systematic reviews and Meta-Analyses extension for Scoping Reviews guidelines to investigate the utility of ICP monitoring as a dynamic predictor of outcomes following TBI. A systematic search of major databases identified relevant studies published between January 1, 1998, and August 1, 2024. Two reviewers identified relevant articles, and conflicts were adjudicated by a third. Data from the included studies were abstracted and synthesized. Analysis of 29 studies (N = 5,743 patients) revealed significant associations between specific ICP patterns and clinical outcomes. Key findings included threshold-dependent mortality predictions, the value of early monitoring patterns (i.e., patterns observed within the first 72 h post-injury), and the enhancement of predictive accuracy through integration with cerebrovascular reactivity indices. Many studies now explore ICP as a multidimensional metric rather than a straightforward number, but overarching conclusions are limited by inter-study variability in analysis. The integration of advanced monitoring techniques, the use of features capturing the temporal complexity of ICP, and machine learning approaches show promise in enhancing the predictive value of ICP monitoring as a new form of precision medicine. These findings support strong associations between specific ICP dynamic patterns and mortality and functional outcomes. Standardization of protocols and validation in diverse populations remain important challenges to address in future studies.

IEEE Trans Cybern (impact factor: 10.5) 1 ☒ TOP

Self Learning Fuzzy Logic-Based Robust Control of Robotic Manipulators Driven With BLDC Motors: A Task Space Control Approach.

Bayram Yilmaz, Sukru Unver, et. al

Abstract:

The primary objective of this study is to enable the end effector of robot manipulators driven by brushless DC motors (BLDC), subjected to model uncertainties, to track the desired trajectory. Direct control in task space, with the primary goal of minimizing the tracking error of the end effector, is favored. Besides, incorporating actuator dynamics (AD) into control synthesis and stability analysis is intended to enhance the sensitivity in terms of positioning and the reliability of robot manipulators. Consideration is given to uncertainties in both the robot manipulator and AD to achieve enhanced tracking performance. In order to improve the efficiency of the closed-loop control system, uncertainties in the dynamic model and AD were estimated using a self-organized adaptive fuzzy logic (AFL) framework, and the obtained estimates were applied to the control torque input. In the employed AFL framework, the means and variances of the membership functions (MFs) are updated online in each iteration, enabling a more accurate estimation of uncertainties. The use of the newly created Lyapunov function demonstrates that the closed-loop system is uniformly ultimately bound. Experimental comparisons were conducted on a two-degree-of-freedom planar robot manipulator driven by a BLDC motor to test the applicability of the presented controller.

IEEE Trans Cybern (impact factor: 10.5) 1 ☒ TOP

New Results on Memory Sampled-Data Control Design for IT2 Fuzzy Singular Systems With External Disturbance.

T Saravanakumar, A Stephen, et al

Abstract:

This work reports design problem of the memory sampled-data (SD) controller for interval type-2 fuzzy singular systems (SSs) with external disturbances. First, an improved free-weighting matrix inequality is introduced for concerning fuzzy SSs to reduce conservatism of the integral terms. Then, a novel looped-functional-based Lyapunov-Krasovskii functional (LKF) is constructed that incorporates the data from sampling interval $z(t)$ to $z(tk)$. With the help of improved integral inequality and novel LKF, a new set of admissibility conditions is developed in the form of linear matrix inequalities (LMIs). The developed criteria based on the memory SD controller ensure that the proposed systems is admissible with an H^∞ attenuation level. Finally, numerical simulations are given to illustrate the usefulness and benefit of the proposed

methods.

Toxics (impact factor: 4.1) 3 ☒

Water Quality Evaluation and Countermeasures of Pollution in Wan'an Reservoir Using Fuzzy Comprehensive Evaluation Model.

Gaoqi Duan, Li Peng, et. al

Abstract:

Water quality evaluation is a crucial component of water source management and pollution prevention, essential for achieving regional water safety and sustainable development. The spatial distribution and trends of major water pollutants in Wan'an Reservoir were analyzed. Subsequently, a fuzzy membership model was employed to develop a comprehensive water quality evaluation method. This approach assessed spatial variations in water quality across the upper, middle, and lower reaches of the reservoir, identifying key factors influencing water quality. The results indicate that water quality in Wan'an Reservoir, primarily characterized by total nitrogen, was poor. Notably, 50% of the sampling points in the main stream were identified as highly polluted, with the highest exceedance rate observed in the middle reaches of the tributaries. Sampling points classified as Class I were predominantly located in the upper reaches, where water quality benefitted from clean incoming water and minimal disturbance. In contrast, the lower reaches experienced more severe pollution due to the cumulative effects of domestic sewage, industrial wastewater, and agricultural runoff. These findings are crucial for developing effective water environmental protection strategies and promoting the sustainable utilization and protection of water resources.

DATA MINING

Front Nutr (impact factor: 5.1) 2 ☒

Risk factors analysis and prediction models of obesity in college students based on dietary patterns.

Jiawang Bai, Mengyuan Chen, et. al

Abstract:

Overweight and obesity among college students have become significant public health concerns. This study aims to develop a nomogram model for assessing obesity risk in college students. A cross-sectional study was conducted among college students in Xuzhou. Demographic, dietary, and lifestyle information was obtained through self-administered questionnaires, while body composition was assessed using the InBody

570 analyzer. Dietary patterns and obesity prevalence were examined through multiple indicators. Principal component analysis (PCA), logistic regression, and a non-invasive risk assessment model based on percentage of body fat (PBF) were applied. The vegetable meat grain dietary pattern and milk egg dietary pattern were associated with a reduced risk of PBF ($P < 0.01$), while the snack mode dietary pattern and aquatic meat dietary pattern increased the risk of PBF ($P < 0.05$). Binary logistic regression identified gender, physical activity, late-night snacking, regular meals, and a healthy diet as key predictors of PBF obesity in college students. The model achieved an area under curve (AUC) of 0.805, with a non-significant Hosmer-Lemeshow (H-L) test ($P > 0.05$). Decision curve analysis (DCA) showed that the model outperformed extreme curves, indicating its reliability. This study highlights the high prevalence of overweight and obesity among college students and the importance of using multiple indicators for comprehensive evaluation. The developed PBF-based nomogram model demonstrates potential for obesity screening but requires further validation in diverse populations. Copyright © 2025 Bai, Chen, Hou, Han, Shao, Zhang, Jiao, Hua and Ren.

Eur J Pharmacol (impact factor: 4.7) 3 ☒

Mapping the Evolving Landscape of Lecanemab Research in Alzheimer's Disease: A Bibliometric Analysis.

Xu Zhao, Ruijia Ma, et. al

Abstract:

Lecanemab, a monoclonal antibody that targets amyloid-beta aggregates, has emerged as a promising therapeutic for Alzheimer's disease (AD). AD is a progressive neurodegenerative disorder characterized by cognitive decline and amyloid pathology. Research on the use of lecanemab in treating AD has increased; however, no relevant bibliometric analyses have been conducted. To address this gap, this study employed bibliometric methods to search for the relevant literature and analyze research trends investigating AD and lecanemab. We performed a literature search of the Web of Science core database for studies investigating AD and lecanemab, published from database inception up to April 3rd, 2025. After rigorous screening, Excel, VOSviewer, and CiteSpace were used to perform a bibliometric analysis of publications, citations, and collaboration networks among countries, institutions, and authors, along with cluster and burst analyses of keywords. Coremine was used for text mining entries significantly related to AD and lecanemab. The number of studies published on AD and lecanemab has increased annually. The countries with the highest publication output were the United States, the United Kingdom, and China. The leading institutions that produced the most articles were Eisai Inc. (Bunkyo City, Tokyo, Japan), Uppsala University (Uppsala, Sweden), and Harvard Medical School (Boston, MA, USA). The top three authors were Lars Lannfelt, Shobha Dhadda, and Michio Kanekiyo. The most prolific journals included The Journal of Alzheimer's Disease, Alzheimer's and Dementia, and Ageing Research Reviews. The most cited article was "Lecanemab in

Early Alzheimer's Disease," by Van Dyck et al., published in The New England Journal of Medicine in 2023, which has accrued 172 citations. The 10 most frequently occurring keywords were Alzheimer's disease, lecanemab, dementia, aducanumab, amyloid-beta, immunotherapy, tau, a-beta, mouse model, and donanemab. Text mining revealed that drugs, anatomical structures, chemical molecules, genes, diseases, and procedures were significantly associated with both AD and lecanemab. The bibliometric and text mining analysis revealed trends in research investigating the correlation between lecanemab and AD. It analyzed the cooperation among countries, regions, and authors, highlighting recent research hotspots. These data offer objective insights for scientific research and clinical practice on lecanemab and AD. These findings provide a roadmap for prioritizing clinical trials, optimizing drug development strategies, and addressing knowledge gaps in amyloid-targeted therapies. Copyright © 2025. Published by Elsevier B.V.

Front Public Health (impact factor: 3.4) 3 

Coping behavior toward occupational health risks among construction workers: determinant identification using the COM-B model and data mining analysis.

Xuesong Yang, Yuyan Ling, et. al

Abstract:

China has the largest construction workforce in the world but faces severe occupational health challenges. Coping behaviors related to occupational health risks (CBOHR) are key to mitigating these hazards but remain understudied. A cross-sectional survey of 484 construction workers was conducted to assess Capability, Opportunity, Motivation, and Behavior using the COM-B model. Structural equation modeling (SEM) was employed to test mediating pathways, and association-rule mining (ARM) was used to identify determinants of high- and low-level CBOHR. The results showed that the COM-B framework-comprising three modules (Capability, Opportunity, and Motivation) with 15 behavior change domains, and a Behavior module with eight specific CBOHRs-demonstrated satisfactory fit, reliability, and validity. Bootstrapping confirmed that Motivation fully mediates the relationship between Capability and Behavior and partially mediates the relationship between Opportunity and Behavior. ARM further identified key domains associated with high and low levels of CBOHR. Strongly correlated item sets identified through association rule analysis revealed domains strongly linked to both high (and low) levels of each CBOHR. This study is the first to integrate the COM-B model with data mining in the context of occupational health, highlighting "motivation-values-policy" as actionable levers for CBOHR interventions. The findings provide preliminary evidence to support the development of scalable worker health programs. Copyright © 2025 Yang, Ling, Wang, Li and Zeng.

IoT

Sensors (Basel) (impact factor: 3.3) 3 

Comparative Performance Analysis of Lightweight Cryptographic Algorithms on Resource-Constrained IoT Platforms.

Tiberius-George Sorescu, Vlad-Mihai Chiriac, et. al

Abstract

The increase in Internet of Things (IoT) devices has introduced significant security challenges, primarily due to their inherent constraints in computational power, memory, and energy. This study provides a comparative performance analysis of selected modern cryptographic algorithms on a resource-constrained IoT platform, the Nordic Thingy:53. We evaluated a set of ciphers including the NIST lightweight standard ASCON, eSTREAM finalists Salsa20, Rabbit, Sosemanuk, HC-256, and the extended-nonce variant XChaCha20. Using a dual test-bench methodology, we measured energy consumption and performance under two distinct scenarios: a low-data-rate Bluetooth mesh network and a high-throughput bulk data transfer. The results reveal significant performance variations among the algorithms. In high-throughput tests, ciphers like XChaCha20, Salsa20, and ASCON32 demonstrated superior speed, while HC-256 proved impractically slow for large payloads. The Bluetooth mesh experiments quantified the direct relationship between network activity and power draw, underscoring the critical impact of cryptographic choice on battery life. These findings offer an empirical basis for selecting appropriate cryptographic solutions that balance security, energy efficiency, and performance requirements for real-world IoT applications.

Sensors (Basel) (impact factor: 3.3) 3 

Development and Evaluation of a Novel IoT Testbed for Enhancing Security with Machine Learning-Based Threat Detection.

Waleed Farag, Xin-Wen Wu, et. al

Abstract

The Internet of Things (IoT) has revolutionized industries by enabling seamless data exchange between billions of connected devices. However, the rapid proliferation of IoT devices has introduced significant security challenges, as many of these devices lack robust protection against cyber threats such as data breaches and denial-of-service attacks. Addressing these vulnerabilities is critical to maintaining the integrity and trust of IoT ecosystems. Traditional cybersecurity solutions often fail in dynamic, heterogeneous IoT environments due to device diversity, limited computational resources, and inconsistent communication protocols, which hinder the deployment of

uniform and scalable security mechanisms. Moreover, there is a notable lack of realistic, high-quality datasets for training and evaluating machine learning (ML) models for IoT security, limiting their effectiveness in detecting complex and evolving threats. This paper presents the development and implementation of a novel physical smart office/home testbed designed to evaluate ML algorithms for detecting and mitigating IoT security vulnerabilities. The testbed replicates a real-world office environment, integrating a variety of IoT devices, such as different types of sensors, cameras, smart plugs, and workstations, within a network generating authentic traffic patterns. By simulating diverse attack scenarios including unauthorized access and network intrusions, the testbed provides a controlled platform to train, test, and validate ML-based anomaly detection systems. Experimental results show that the XGBoost model achieved a balanced accuracy of up to 99.977% on testbed-generated data, comparable to 99.985% on the benchmark IoT-23 dataset. Notably, the SVM model achieved up to 96.71% accuracy using our testbed data, outperforming its results on IoT-23, which peaked at 94.572%. The findings demonstrate the testbed's effectiveness in enabling realistic security evaluations and ability to generate real-world datasets, highlighting its potential as a valuable tool for advancing IoT security research. This work contributes to the development of more resilient and adaptive security frameworks, offering valuable insights for safeguarding critical IoT infrastructures against evolving threats.

EVOLUTIONARY COMPUTING

ACS Omega (impact factor: 4.3) 3 

Optimizing Multi-Task Learning with Evolutionary Relatedness Metrics for Enhanced QSAR-Based Natural Product Activity Prediction.

Donny Ramadhan, Reiko Watanabe, et. al

Abstract

Natural products exhibit diverse and typically nonflat structures, which could be essential in drug-target interactions. Given limited bioactivity data for natural products in public databases, multitask learning (MTL) offers a promising strategy to improve quantitative structure-activity relationship (QSAR)-based predictions. This study optimized MTL with evolutionary relatedness metrics of proteins to enhance the prediction of natural product bioactivity, particularly when data are scarce, and identified conditions under which MTL is most effective. A curated data set of predicted natural products with bioactivity against enzymes from ChEMBL was constructed using binary classification filtering. Single-task learning (STL) served as the baseline, feature-based MTL (FBMTL) was applied across all proteins within each protein group, and instance-based MTL (IBMTL), a variant of FBMTL, incorporated evolutionary

relatedness metrics. IBMTL outperformed STL and FBMTL across most protein groups, suggesting that evolutionary relatedness improves performance. Significant improvements were observed in the kinase and cytochrome P450 protein groups, whose proteins are classified at more specific levels of ChEMBL's 6-level hierarchical protein classification. In the kinase group, IBMTL performed best at the target parent level, highlighting a trade-off between relatedness and data set size. This study demonstrates the potential of MTL in natural product-based drug discovery by leveraging evolutionary relatedness despite limited data availability. © 2025 The Authors. Published by American Chemical Society.

ACS Omega (impact factor: 4.3) 3 

Molecular Paleontology Meets Drug Discovery: The Case for De-extinct Antimicrobials.

Rumiana Tenchov, Qiongqiong Zhou, et. al

Abstract:

The rise of antibiotic resistance has necessitated the exploration of unconventional sources of novel antimicrobial agents. One emerging novel frontier is "de-extinct" molecules—bioactive peptides, antibiotics, and other bioactive agents reconstructed from ancient or extinct organisms—an innovative convergence of paleogenomics, paleoproteomics, and synthetic biology. Recent advances in high-throughput DNA sequencing, mass spectrometry, and computational biology have enabled scientists to recover and analyze genetic and protein sequences from long-extinct species, offering unprecedented insights into evolutionary biology and potential applications in medicine, biotechnology, and conservation, including the successful regeneration of antimicrobial molecules from several extinct organisms. While paleogenomics provides the blueprint for reconstructing extinct genomes, paleoproteomics offers complementary insights into gene expression, protein function, and post-translational modifications that are often lost in DNA-based studies. These approaches can yield proteins and metabolites that have been lost to evolution, offering a new reservoir of bioactive compounds that could be used for new strategies in medicine, biotechnology, and synthetic biology. In this report we explore data from the CAS Content Collection to outline the current landscape and research progress in the emerging area of molecular de-extinction, to identify key developing concepts and challenges, and to identify successfully revived de-extinct antimicrobials. We outline the technical approaches to their revival in an effort to understand how this highly innovative strategy helps combat modern multidrug-resistant pathogens as well as the challenges and ethical considerations in deploying ancient molecules. © 2025 The Authors. Published by American Chemical Society.

PNAS Nexus (impact factor: 3.8) 3 

Welfare optimization for resource allocation with peer effects.

Zirou Qiu, Daniel Rosenkrantz, et. al

Abstract:

Allocating students to schools or universities, people to teams or groups, people to urban housing, and matching users on social platforms are prominent examples of allocating limited goods, spaces, or positions to optimize social welfare. We study a welfare maximization problem that arises when such resource allocation scenarios involve peer effects, where people have preferences over the others who are nearby (e.g. their classmates, teammates, neighbors, or partners). We first develop a unified mathematical framework for this "position allocation problem," which assigns people to positions in a given network, with people caring about both their positions and their neighbors' attributes. We show that welfare maximization for the corresponding position allocation problem is computationally intractable, even when people have preferences that depend only on who is allocated to nearby positions, and those preferences satisfy simple constraints that arise naturally in urban and other real-world systems. In contrast to this computational lower bound, we show that if people can be classified into a fixed number of (demographic) groups and the network satisfies certain realistic spatial conditions, then efficiently computable allocations can be obtained for many natural scenarios. Importantly, the achieved social welfare is either optimal or arbitrarily close to optimal for natural forms of preferences. Our methods provide a foundation for position allocation with peer effects, and guide the design of optimal allocation strategies when people can be classified into a fixed number of groups in which members share similar preferences. Published by Oxford University Press on behalf of National Academy of Sciences 2025. 748

II Concentration

PHYSICS

Directly observing replica symmetry breaking in a vector quantum-optical spin glass

Ronen M. Kroeze, Brendan P. Marsh, et al.

Abstract

Spin glasses are quintessential examples of complex matter. Although their ordering lacks complete theoretical understanding, abstract models of spin glasses inform problems in other fields, such as combinatorial optimization and artificial intelligence—where they form a mathematical basis for neural network computing. We demonstrate the ability to realize a spin glass of a distinct driven-dissipative and vector form. By microscopically visualizing its glassy spin states, the technique allows us to directly measure replica symmetry breaking and the resulting ultrametric hierarchical structure. Ultrametricity is known to be emergent in models of evolution, protein folding, and climate change; this work shows it to be directly observable in a physically realized system.

Probing the Kitaev honeycomb model on a neutral-atom quantum computer

Evered, Simon J., Kalinowski, et al.

Abstract

Quantum simulations of many-body systems are among the most promising applications of quantum computers¹. In particular, models based on strongly correlated fermions are central to our understanding of quantum chemistry and materials problems², and can lead to exotic, topological phases of matter^{3,4}. However, owing to the non-local nature of fermions, such models are challenging to simulate with qubit devices⁵. Here we realize a digital quantum simulation architecture for two-dimensional fermionic systems based on reconfigurable atom arrays⁶. We utilize a fermion-to-qubit mapping based on Kitaev's model on a honeycomb lattice³, in which fermionic statistics are encoded using long-range entangled states⁷. We prepare these states efficiently using measurement⁸ and feedforward⁹, realize subsequent fermionic evolution through Floquet engineering^{10,11} with tunable entangling gates¹² interspersed with atom rearrangement, and improve results with built-in error detection. Leveraging this fermion description of the Kitaev spin model, we efficiently prepare topological states across its complex phase diagram¹³ and verify the non-Abelian spin-liquid phase³ by

evaluating an odd Chern number^{14,15}. We further explore this two-dimensional fermion system by realizing tunable dynamics and directly probing fermion exchange statistics. Finally, we simulate strong interactions and study the dynamics of the Fermi–Hubbard model on a square lattice. These results pave the way for digital quantum simulations of complex fermionic systems for materials science, chemistry¹⁶ and high-energy physics¹⁷.

Probing non-equilibrium topological order on a quantum processor

Will, M., Cochran, T. A., Rosenberg, et al.

Abstract

Out-of-equilibrium phases in many-body systems constitute a new paradigm in quantum matter—they exhibit dynamical properties that may otherwise be forbidden by equilibrium thermodynamics. Among these non-equilibrium phases are periodically driven (Floquet) systems, which are generically difficult to simulate classically because of their high entanglement. Here we realize a Floquet topologically ordered state theoretically proposed in ref. 6, on an array of superconducting qubits. We image the characteristic dynamics of its chiral edge modes and characterize its emergent anyonic excitations. Devising an interferometric algorithm allows us to introduce and measure a bulk topological invariant to probe the dynamical transmutation of anyons for system sizes up to 58 qubits. Our work demonstrates that quantum processors can provide key insights into the thus-far largely unexplored landscape of highly entangled non-equilibrium phases of matter.

MATERIALS

Dual-scale chemical ordering for cryogenic properties in CoNiV-based alloys

Lu, Tiwen, Sun, et al.

Abstract

The mechanical properties of metallic materials often degrade under harsh cryogenic conditions, posing challenges for low-temperature infrastructures¹. Here we introduce a dual-scale atomic-ordering nanostructure, characterized by an exceptionally high number density of co-existing subnanoscale short-range ordering (approximately $2.4 \times 10^{26} \text{ m}^{-3}$) and nanoscale long-range ordering (approximately $4.5 \times 10^{25} \text{ m}^{-3}$) domains, within a metallic solid-solution matrix in a CoNiV-based alloy

to improve the synergy of strength and ductility at low temperatures. We observe an ordering-induced increase in dislocation shear stress as well as a more rapid dislocation multiplication owing to the dislocation blocking effect of nanoscale long-range ordering and the associated generation of new dislocations. The latter effect also releases stress concentrations at nanoscale long-range-ordered obstacles that otherwise would promote damage initiation and failure. Consequently, the alloy shows a strength–elongation product of 76 GPa % with a yield strength of approximately 1.2 GPa at 87 K, outperforming materials devoid of such ordering hierarchy, containing only short-range ordered or coherent precipitates of a few tens of nanometres. Our results highlight the impact of dual co-existing chemical ordering on the mechanical properties of complex alloys and offer guidelines to control these ordering states to enhance their mechanical performance for cryogenic applications.

Rapid, low-temperature nanodiamond formation by electron-beam activation of adamantane C–H bonds

Jiarui Fu, Takayuki Nakamuro, et al.

Abstract

Diamond and adamantane (Ad) share a Td-symmetric carbon skeleton, but converting Ad to diamond has been challenging because it requires selective carbon-hydrogen (C–H) bond cleavage and monomer assembly into a diamond lattice. Our approach differs from the conventional high-temperature, high-pressure diamond syntheses. We electron-irradiated Ad submicrocrystals at 80 to 200 kilo–electron volts and 100 to 296 kelvin in vacuum for tens of seconds. This process yielded defect-free nanodiamonds (NDs) of cubic crystal structure, accompanied by hydrogen gas evolution. Time-resolved transmission electron microscopy revealed the initial formation of Ad oligomers transforming into spherical NDs. A sizable kinetic isotope effect indicates that C–H cleavage was rate-determining, and other hydrocarbons tested failed to form NDs.

Spin-selective transport through chiral ferromagnetic nanohelices

Yoo Sang Jeon, Eunjin Jeong, et al.

Abstract

Chiral crystals with well-defined handedness in atomic arrangements exhibit properties such as spin selectivity, asymmetric magnetoresistance, and skyrmions. Although similar geometry-induced phenomena in chiral organic molecule-based systems were observed, synthesizing uniform inorganic nanostructures with desired chirality using a scalable method remains challenging. We electrochemically synthesized chiral ferromagnetic cobalt-iron nanohelices from nanoparticles in anodized aluminum oxide

templates. The spiral directions and the number of strands were regulated by incorporating chiral molecules and applying an appropriate potential. We demonstrate the observation of Faraday's law of induction at the nanoscale and show how chiral nanohelices regulate the electron flow direction. The implications of our findings extend to the technological realm, with chirality- and ferromagnetism-based spin-tunable devices.

CHEMISTRY

Microcanonical kinetics of water-mediated proton transfer in microhydrated 4-aminobenzoic acid

Abhijit Rana, Payten A. Harville, et. al

Abstract

Isolated cluster systems can help to elucidate the molecular level description of water-mediated proton transfer. Protonation of neutral 4-aminobenzoic acid (4ABA) occurs at the acid (*O*-protomer) and amine (*N*-protomer) functionalities, yielding two distinct species with relative energies dependent on the degree of hydration. Here, we measured the rates of intramolecular proton transfer in $4\text{ABAH}^+(\text{H}_2\text{O})_6$ ions upon protomer-selective vibrational excitation of initially cold (6 K) cluster ions isolated in a cryogenic ion trap. Interconversion rates were observed on the microsecond time scale. These results quantify the kinetics of proton transfers in the context of a closed, finite system at well-defined internal energies and therefore provide experimental benchmarks for theoretical efforts that are being developed to treat relatively slow, highly cooperative solvent-mediated chemical processes.

A main-group metal carbonyl complex: Structure and isomerization to a carbene-stabilized tin atom

Maximilian Dietz, Andrey V. Protchenko, et. al

Abstract

In contrast to transition elements, s- and p-block metal compounds that coordinate carbon monoxide (CO) under near-ambient conditions are elusive. Here, we report an isolable, crystalline main-group metal carbonyl complex and its isomerization to a carbene-stabilized metal atom. The stannylene (Boryl)₂Sn [where Boryl is B(NDippCH)₂] coordinates CO reversibly, affording an isolable adduct below 0°C, which was characterized by x-ray crystallography. This complex rearranges at

temperatures above 0°C to generate the stannavinylidene, (Boryl)(OBoryl)C=Sn, that is, a complex between the triplet carbene (Boryl)(OBoryl)C and monatomic Sn(0) in its electronic ground state.

Photochemical H₂ dissociation for nearly quantitative CO₂ reduction to ethylene

Ping Jin, Pu Guo, et. al

Abstract

Producing olefins by carbon dioxide (CO₂) hydrogenation is a long-standing goal. The usual products are multicarbon mixtures because the critical step of heterolytic hydrogen (H₂) dissociation at high temperatures complicates selectivity control. In this study, we report that irradiating gold–titanium dioxide at 365 nanometers induces heterolytic H₂ dissociation at ambient temperature. This process likely relies on interfacial electric dipoles from photogenerated electrons and holes situated on the metallic gold nanoparticles and interfacial gold–oxygen–titanium scaffolds. The heterolytic H₂ dissociation is further promoted by light-induced coating of gold nanoparticles with a titanium oxide layer. The resulting nucleophilic hydrogen species reduce CO₂ to ethane in >99% yield under light irradiation in a flow apparatus. Furthermore, cascading with a subsequent photocatalytic ethane dehydrogenation generates ethylene in >99% yield over 1500 hours of irradiation.

BIOLOGY

Oxytocin signaling regulates maternally directed behavior during early life

Daniel D. Zelmanoff, Rebecca Bornstein, et al.

Abstract

Oxytocin is essential in shaping social behavior across the lifespan. Although the role of oxytocin signaling in parental care has been widely investigated, little is known about its function in social behavior during early life. We studied the role of oxytocin in mouse pup social behavior during acute separation from the mother as well as upon reunion. The activity of oxytocin neurons was increased by acute maternal separation. Behaviorally, maternally separated pups emitted more ultrasonic vocalizations upon reunion, which were further modulated by nipple attachment behavior. These effects were attenuated by blocking the oxytocin receptor during maternal separation. Optogenetic silencing of oxytocin neurons during maternal separation disrupted vocal

behavior during separation and reunion. Our findings reveal an important role of oxytocin in context-dependent vocal communication in mouse pups.

Dual-cycle CO₂ fixation enhances growth and lipid synthesis in *Arabidopsis thaliana*

Kuan-Jen Lu, Chia-Wei Hsu, et. al

Abstract

Carbon fixation through the Calvin-Benson-Bassham (CBB) cycle accounts for the majority of carbon dioxide (CO₂) uptake from the atmosphere. The CBB cycle generates C₃ carbohydrates but is inefficient at producing acetyl-coenzyme A (CoA) (C₂), which is the universal precursor for synthesizing lipids. In this work, we introduced in *Arabidopsis thaliana* a new-to-nature CO₂ fixing cycle, malyl-CoA-glycerate (McG) cycle, which together with the CBB cycle forms a dual-cycle CO₂ fixation system. This cycle can fix one additional carbon by phosphoenolpyruvate carboxylase and convert the photorespiration product, glycolate, to acetyl-CoA. Plants with the McG cycle show enhanced protein abundance in their photosystems and enhanced photosystem II efficiency. McG plants had doubled CO₂ fixation rates under atmospheric CO₂, increased lipid production, pronounced growth enhancement, and tripled the seed yield.

Visual objects refine head direction coding

Dominique Siegenthaler, Henry Denny, et. al

Abstract

Animals use visual objects to guide navigation-related behaviors. However, visual object-prefering areas have yet to be described in the mouse brain, limiting our understanding of how visual objects affect spatial navigation system processing. Using functional ultrasound imaging, we identified brain areas that were preferentially activated by images of objects compared with their scrambled versions. Whereas visual cortex did not show a preference, areas associated with spatial navigation were preferentially activated by visual objects. Electrophysiological recordings in postsubiculum, the cortical head direction (HD) system hub, confirmed a preference for visual objects in both HD cells and fast-spiking interneurons. In freely moving animals, visual objects increased firing rates of HD cells aligned with a visual object but decreased activity in HD cells coding for other directions.

III Calling for papers

ICCDC 2025 (EI)

Submission deadline: Oct 10, 2025
Conference date: Oct 31, 2025 - Nov 2, 2025
Full name: 2025 International Conference on Computer Technology, Digital Media, and Communication
Location: Chengdu, China

2025 International Conference on Computer Technology, Digital Media, and Communication (ICCDC 2025) will be held in 2025, providing a platform for global scholars, researchers, and industry experts to exchange ideas and foster collaboration. As information technology advances at an unprecedented pace, the fields of computer technology, digital media, and communication face both remarkable opportunities and significant challenges. Emerging technologies such as artificial intelligence, big data, and virtual reality are profoundly transforming how people live and communicate. Therefore, it is crucial to explore these innovations and their impacts on society, culture, and the economy.

The primary goal of ICCDC 2025 is to bring together experts and scholars from around the world to share the latest research findings, technological innovations, and practical applications, thereby promoting close ties between academia and industry. The conference will feature keynote speeches, paper presentations, panel discussions, and interactive workshops, addressing cutting-edge topics across computer science, digital media arts, communication studies, and related interdisciplinary fields. We invite researchers to submit their contributions and collaborate on advancing this dynamic domain, fostering the dissemination of knowledge and the sparks of innovation.

Call for papers:

- Track 1: Digital Media Technology and Generative AI
 - Deep Learning
 - Image Generation
 - Video Generation
 - Data Augmentation
 - Augmented Reality
 - Virtual Reality
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- Track 2: Digital Communication Technology
 - Image Enhancement
 - Image Editing
- Track 3: Information Security
 - Image Compression
 - Data Compression and Transmission
 - Big Data Signal Processing
 -
 - Generative Adversarial Networks
 - Generative Modeling Techniques
 - Language Pre-training
 - Visual Pre-training
 - Joint Pre-training
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ICSIM 2026 (EI)

Submission deadline: Oct 10, 2025
Conference date: Jan 21, 2026 - Jan 23, 2026
Full name: The 9th International Conference on Software Engineering and Information Management
Location: Yokohama, Japan

ICSIM 2026 > Home

The Organizing Committee is pleased to announce that the 2026 The 9th International Conference on Software Engineering and Information Management (ICSIM 2026) will be held in Yokohama, Japan, on January 21-23, 2026. ICSIM 2026 will be proudly sponsored by Keio University, one of Japan's most prestigious institutions, renowned for its excellence in research and education in the fields of technology and management.

Yokohama, a vibrant and dynamic city located just south of Tokyo, is known for its rich history, stunning waterfront views, and cutting-edge technological innovations. As one of Japan's major ports and a hub for international business, Yokohama provides an ideal setting for the conference, combining modernity with tradition. The city is home to numerous tech startups, research facilities, and cultural landmarks, making it an inspiring place for academics and professionals to exchange ideas and discuss the latest trends in software engineering and information management.

ICSIM was initiated in Casablanca, Morocco in 2018, and has since been held in Bali, Indonesia (2019), Sydney, Australia (2020), Yokohama, Japan virtually (2021-2022) due to the impact of the COVID-19 pandemic, Palmerston North, New Zealand (2023), Fiji (online) in 2024, and Singapore in 2025. The conference has grown year after year, attracting a diverse range of participants from around the world.

Topics of Interest :

The topics of interest for submission include, but are not limited to:

Track 1: Advanced Software Engineering and Development

- *Software Architecture and Design Patterns
- *Agile Development and DevOps Practices
- *Software Testing, Verification and Validation
- *Requirements Engineering and Management

Track 2: Intelligent Systems and Emerging Technologies

- *AI-Assisted Software Engineering
- *Machine Learning in Software Development
- *Natural Language Processing Applications
- *Intelligent Agents and Multi-Agent Systems

Track 3: Information Systems and Data Engineering

- *Data Mining and Knowledge Discovery
- *Big Data Analytics and Infrastructure

- *Information Retrieval and Search Technologies
- *Cloud Computing and Edge Intelligence

Track 4: Communication and Cyber-Physical Systems

- *Wireless and Mobile Communication Systems
- *Next-Generation Network Architecture (5G/6G)
- *IoT and Embedded Systems
- *Cyber-Physical Systems and Industrial IoT

Track 5: Software Process and Digital Transformation

- *Software Process Improvement and Maturity Models
- *DevOps Pipelines and Toolchains
- *Software Project Management and Cost Estimation
- *Reengineering and Reverse Engineering

Track 6: Security, Ethics, and Societal Impact

- *Information and Cyber Security
- *Software and Data Privacy Engineering
- *AI Ethics and Responsible Computing
- *Risk Analysis and Safety-Critical Systems

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AIPIP 2025 (IEEE-EI/SCOPUS)

Submission deadline: Oct 10, 2025
Conference date: Oct 17, 2025 - Oct 19, 2025
Full name: International Conference on Aerospace Information Perception and Intelligent Processing
Location: Shenyang, China

About AIPIP 2025

2025 International Conference on Aerospace Information Perception and Intelligent Processing
2025 International Conference on Aerospace Information Perception and Intelligent Processing (AIPIP 2025) will be grandly held in Shenyang, China, from October 17 to 19, 2025.

This event will unite researchers, engineers, industry experts, and practitioners worldwide to discuss the latest advancements in aerospace information perception and intelligent processing. As technology in aerospace rapidly evolves, the significance of sophisticated data analysis, machine learning, and artificial intelligence in enhancing aerial operations has grown immensely. AIPIP 2025 will offer an engaging platform for participants to share their research findings through keynote speeches, oral report, and poster presentation. Key topics will include sensor technologies, image processing, autonomous systems, and intelligent decision-making processes in aerospace

applications.

The conference aims to promote interdisciplinary collaboration by inviting contributions from aerospace engineering, computer science, and information technology. Attendees will have numerous opportunities to network and exchange ideas, paving the way for future innovations in aerospace technology. We are excited to welcome you to Shenyang for an inspiring conference experience at AIPIP 2025, where tradition meets cutting-edge innovation.

Call for Papers:

**** (1) Aerospace Information Sensing ****: Sensor technology, remote sensing technology, radar detection technology, aerospace information acquisition technology, Earth observation technology, near-space sensing technology, and space situational awareness technology;

**** (2) Aerospace Information Transmission ****: Aerospace communication, drone communication, integrated aerospace command and control technology, millimeter-wave and terahertz communication technology, semantic communication technology, airborne intelligent networking technology, intelligent resource allocation technology, large-scale bionic communication network technology, and anti-jamming communication technology;

**** (3) Intelligent Processing of Aerospace Information ****: Hyperspectral information processing technology, microwave imaging technology, radar imaging technology, multisource information fusion technology, multimodal signal processing technology, aerospace information compression technology, navigation technology, big data technology, and artificial intelligence technology;

**** (4) Intelligent Application of Aerospace Information ****: Electromagnetic information control and effects, electromagnetic compatibility, flight control, mission planning, hardware-in-the-loop simulation, reliability analysis, fault diagnosis, unmanned systems, intelligent processing of satellite navigation information, multisource integrated navigation enhancement, anti-jamming/deception navigation technology, and smart aerospace information applications;

**** (5) Integration of Aerospace Information Industry ****: Low-altitude economy, commercial aerospace, deep space exploration, satellite applications, digital earth, and next-generation information technology.....

ISPDS 2025 (IEEE)

Submission deadline: Oct 10, 2025
Conference date: Oct 31, 2025 - Nov 2, 2025
Full name: 6th International Conference on Information Science, Parallel and Distributed Systems
Location: London, United Kingdom

The 6th International Conference on Information Science, Parallel and Distributed Systems (ISPDS 2025) is scheduled to be held in London, U.K. from October 31 to November 2, 2025. The conference aims to provide a platform for experts and scholars engaged in information science,

parallel or distributed processing research, engineering and technical personnel, and technology research and development personnel to share scientific research results and cutting-edge technologies, understand academic development trends, broaden research ideas, strengthen academic research and discussion, and promote the industrialization of academic achievements. The conference sincerely invites experts, scholars from domestic and foreign universities, research institutions, business people and other relevant personnel to participate in the exchange.

***Call for papers:**

- Algorithms
- Artificial Intelligence
- Applications
- Compilers and runtime systems
- Communication
- Deep memory hierarchies
- Development, analysis, or management tools
- Data Compression
- Data Mining
- Data Engineering
- Fault tolerance for Parallel and Distributed systems
- High performance computing, cloud and grid computing
- Information Retrieval
- Image Processing
- Information Systems
- Middleware and Software engineering
- Programming languages
- Programming theory and models
- Security in Computing
- Signal Processing
- Wireless and Mobile Computing

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AISNS 2025

Submission deadline: Oct 13, 2025
Conference date: Nov 14, 2025 - Nov 16, 2025
Full name: 3rd International Conference on Artificial Intelligence, Systems and Network Security
Location: Xiangtan,China

2025 3rd International Conference on Artificial Intelligence, Systems and Network Security

(AISNS 2025) will be held on November 14-16, 2025 in Xiangtan, China.

AISNS 2025 is to bring together innovative academics and industrial experts in the field of Artificial Intelligence, Systems and Cyber Security to a common forum. The primary goal of the conference is to promote research and developmental activities in computer information science and application technology and another goal is to promote scientific information interchange between researchers, developers, engineers, students, and practitioners working all around the world. The conference will be held every year to make it an ideal platform for people to share views and experiences in computer information science and application technology and related areas.

Topics of interest

1. Artificial Intelligence

- AI Algorithms
- Natural Language Processing
- Fuzzy Logic
- Computer Vision and Image Understanding
- Signal and Image Processing
- Speech and Natural Language Processing
- Computational Theories of Learning
- Information Retrieval and Fusion
- Hybrid Intelligent Systems
- Intelligent System Architectures
- Knowledge Representation
- Knowledge-based Systems
- Mechatronics
- Database Systems
- Network Systems
- Compilation Systems
- Computer Architecture
- Virtualization Technology
- Container Technology

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2. Network Security

- Active Defense Systems
- Adaptive Defense Systems
- Analysis, Benchmark of Security Systems
- Applied Cryptography
- Authentication
- Biometric Security
- Complex Systems Security
- Database and System Security
- Data Protection
- Data/System Integrity
- Distributed Access Control
- Distributed Attack Systems

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3. Computer Systems

- Operating Systems
- Distributed Systems