Science Newsletter

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Contents

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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/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 **Mathematics**:
We post several papers which are related to the top concerned topics in researches on Mathematics. The papers are classified in 5 categories, and they are: **Topology, Discrete Mathematics, Optimization, Applied Partial Differential Equations** and **Nonlinear stability theory**. 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.

TOPOLOGY

Science (impact factor: 56.9) 1 区 TOP

Mapping twist-tuned multiband topology in bilayer WSe2.

Foutty, Kometter, et. al

Abstract:
Semiconductor moiré superlattices have been shown to host a wide array of interaction-driven ground states. However, twisted homobilayers have been difficult to study in the limit of large moiré wavelengths, where interactions are most dominant. In this study, we conducted local electronic compressibility measurements of twisted bilayer WSe2 (tWSe2) at small twist angles. We demonstrated multiple topological bands that host a

series of Chern insulators at zero magnetic field near a "magic angle" around 1.23°. Using a locally applied electric field, we induced a topological quantum-phase transition at one hole per moiré unit cell. Our work establishes the topological phase diagram of a generalized Kane-Mele-Hubbard model in tWSe2, demonstrating a tunable platform for strongly correlated topological phases.

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

Leveraging Bilateral Correlations for Multi-Label Few-Shot Learning.

An, Xue, et. al

Abstract:

Multi-label few-shot learning (ML-FSL) refers to the task of tagging previously unseen images with a set of relevant labels, giving a small number of training examples. Modeling the correlations between instances and labels, formulated in the existing methods, allows us to extract more available knowledge from limited examples. However, they simply explore the instance and label correlations with a uniform importance assumption without considering the discrepancy of importance in different instances or labels, making the utilization of instance and label correlations a bottleneck for ML-FSL. To tackle the issue, we propose a unified framework named bilateral correlation reconstruction (BCR) to enable the network to effectively mine underlying instance and label correlations with varying importance information from both instance-to-label and label-to-instance perspectives. Specifically, from the instance-to-label perspective, we refine prototypes per category by reweighting each image with its specific instance-importance degree extracted from the similarity between the instance and the corresponding category. From the label-to-instance perspective, we smooth labels for each image by recovering latent label-importance with considering the integrated topology of all samples in a task. Experimental results on multiple benchmarks validate that BCR could outperform existing ML-FSL methods by large margins.

J Chem Theory Comput (impact factor: 5.5) 1 区

Efficient Generation of Conformer Ensembles Using Internal Coordinates and a Generative Directional Graph Convolution Neural Network.

Raush, Abagyan, et. al

Abstract:

We present a neural-network-based high-throughput molecular conformer-generation algorithm. A chemical graph-convolutional network is trained to predict low-energy conformers in internal coordinate representation (bond lengths, bond, and torsion angles), starting from two-dimensional (2D) chemical topology. Generative neural network (NN) architecture performs denoising from torsion space, producing

conformer ensembles with populations that are well correlated with torsion energy profiles. Short force-field-based energy minimization is applied to refine final conformers. All computation-intensive stages of the algorithm are GPU-optimized. The procedure (termed GINGER) is benchmarked on a commonly used test set of bioactive three-dimensional (3D) conformers from the PDB. We demonstrate highly competitive results in conformer recovery and throughput rates suitable for giga-scale compound library processing. A web server that allows interactive conformer ensemble generation by GINGER and their viewing is made freely available at https://www.molsoft.com/gingerdemo.html.

DISCRETE MATHEMATICS

Adv Sci (Weinh) (impact factor: 15.8) 1 区

Tumor Biomechanics Alters Metastatic Dissemination of Triple Negative Breast Cancer via Rewiring Fatty Acid Metabolism.

Filipe, Velayuthar, et. al

Abstract:
In recent decades, the role of tumor biomechanics on cancer cell behavior at the primary site has been increasingly appreciated. However, the effect of primary tumor biomechanics on the latter stages of the metastatic cascade, such as metastatic seeding of secondary sites and outgrowth remains underappreciated. This work sought to address this in the context of triple negative breast cancer (TNBC), a cancer type known to aggressively disseminate at all stages of disease progression. Using mechanically tuneable model systems, mimicking the range of stiffness's typically found within breast tumors, it is found that, contrary to expectations, cancer cells exposed to softer microenvironments are more able to colonize secondary tissues. It is shown that heightened cell survival is driven by enhanced metabolism of fatty acids within TNBC cells exposed to softer microenvironments. It is demonstrated that uncoupling cellular mechanosensing through integrin β1 blocking antibody effectively causes stiff primed TNBC cells to behave like their soft counterparts, both in vitro and in vivo. This work is the first to show that softer tumor microenvironments may be contributing to changes in disease outcome by imprinting on TNBC cells a greater metabolic flexibility and conferring discrete cell survival advantages.

Spectrochim Acta A Mol Biomol Spectrosc (impact factor: 4.4) 2 区

New approach for near-infrared wavelength selection using a combination of MIC and firefly evolution.

Hong, Zhang, et al

Abstract:

Full-length spectral data analysis has a big problem that the variables are highly in collinearity and correlation. Spectral wavelength selection is a continuing hot topic in quantitative or qualitative analysis. In this paper, we propose a new approach for near-infrared (NIR) wavelength selection. The novel strategy mainly refers to the modification of maximum information coefficient (MIC) method and an improvement of firefly evolutionary algorithm. We introduce the orthogonal decomposition to modify the MIC method, so as to search the informative signals conceived in projection vectors. We also raise the common firefly algorithm (FA) as in the discretized mode, and design a novel adaptive mapping function to improve its intelligent computing effect. In experiment, the modified MIC (MICm) method and the adaptive discrete FA algorithm (DFAadp) are joint together for combined optimization of the NIR calibration model. The proposed combined modeling strategy is applied for quantitative analysis of the fishmeal samples, in the concern to select their informative variables/wavelengths. Experimental results indicate that the combination of MICm and DFAadp perform better than traditional MIC method and common DFA. We conclude that the proposed combined optimization strategy is beneficial for wavelength selection in NIR spectral analysis. It is anticipated to be validated for further applications in a wide range.

PLoS Comput Biol (impact factor: 4.3) 2 区 TOP

HGCLAMIR: Hypergraph contrastive learning with attention mechanism and integrated multi-view representation for predicting miRNA-disease associations.

Ouyang, Liang, et. al

Abstract:

Existing studies have shown that the abnormal expression of microRNAs (miRNAs) usually leads to the occurrence and development of human diseases. Identifying disease-related miRNAs contributes to studying the pathogenesis of diseases at the molecular level. As traditional biological experiments are time-consuming and expensive, computational methods have been used as an effective complement to infer the potential associations between miRNAs and diseases. However, most of the existing computational methods still face three main challenges: (i) learning of high-order relations; (ii) insufficient representation learning ability; (iii) importance learning and integration of multi-view embedding representation. To this end, we developed a HyperGraph Contrastive Learning with view-aware Attention Mechanism and Integrated multi-view Representation (HGCLAMIR) model to discover potential miRNA-disease associations. First, hypergraph convolutional network (HGCN) was utilized to capture high-order complex relations from hypergraphs related to miRNAs and diseases. Then, we combined HGCN with contrastive learning to improve and enhance the embedded representation learning ability of HGCN. Moreover, we introduced view-aware attention mechanism to adaptively weight the embedded representations of different views, thereby obtaining the importance of multi-view latent representations. Next, we innovatively proposed integrated representation learning to integrate the embedded representation information of multiple views for obtaining more reasonable embedding information. Finally, the integrated representation information was fed into a neural network-based matrix completion method to perform miRNA-disease association prediction. Experimental results on the cross-validation set and independent test set indicated that HGCLAMIR can achieve better prediction performance than other baseline models. Furthermore, the results of case studies and enrichment analysis further demonstrated the accuracy of HGCLAMIR and unconfirmed potential associations had biological significance.

OPTIMIZATION

Adv Mater (impact factor: 29.4) 1 区 TOP

Co-assembled Nanoparticles Towards Multi-target Combinational Therapy of Alzheimer's Disease by Making Full Use of Molecular Recognition and Self-assembly.

Li, Xu, Wang, et. al

Abstract:

The complex pathologies in Alzheimer's disease (AD) severely limits the effectiveness of single-target pharmic interventions, thus necessitating multi-pronged therapeutic strategies. While flexibility is essentially demanded in constructing such multi-target systems, for achieving optimal synergies and also accommodating the inherent heterogeneity within AD. Utilizing the dynamic reversibility of supramolecular strategy for conferring sufficient tunability in component substitution and proportion adjustment, amphiphilic calixarenes are poised to be a privileged molecular tool for facilely achieving function integration. Herein, taking β-amyloid (Aβ) fibrillation and oxidative stress as model combination pattern, we proposed a supramolecular multifunctional integration by co-assembling guanidinium-modified calixarene with ascorbyl palmitate and loading dipotassium phytate within calixarene cavity. Serial pivotal events can be simultaneously addressed by this versatile system, including (1) inhibition of Aβ production and aggregation, (2) disintegration of Aβ fibrils, (3) acceleration of Aβ metabolic clearance, and (4) regulation of oxidative stress, which is verified to significantly ameliorate the cognitive impairment of 5×FAD mice, with reduced Aβ plaque content, neuroinflammation and neuronal apoptosis. Confronted with the extremely intricate clinical realities of AD, the strategy presented here exhibits ample adaptability for necessary alterations on combinations, thereby may immensely expedite the advancement of AD combinational therapy through providing an exceptionally convenient platform.

J Agric Food Chem (impact factor: 6.1) 1 区 TOP

Design, Synthesis, Antibacterial Activity, and Mechanisms of Novel Benzofuran Derivatives Containing Disulfide Moieties.

Li, Liu, Li, et. al

Abstract:

The unsatisfactory effects of conventional bactericides and antimicrobial resistance have increased the challenges in managing plant diseases caused by bacterial pests. Here, we report the successful design and synthesis of benzofuran derivatives using benzofuran as the core skeleton and splicing the disulfide moieties commonly seen in natural substances with antibacterial properties. Most of our developed benzofurans displayed remarkable antibacterial activities to frequently encountered pathogens, including Xanthomonas oryzae pv oryzae (Xoo), Xanthomonas oryzae pv oryzicola (Xoc), and Xanthomonas axonopodis pv citri (Xac). With the assistance of the three-dimensional quantitative constitutive relationship (3D-QSAR) model, the optimal compound V40 was obtained, which has better in vitro antibacterial activity with EC50 values of 0.28, 0.56, and 10.43 μg/mL against Xoo, Xoc, and Xac, respectively, than those of positive control, TC (66.41, 78.49, and 120.36 μg/mL) and allicin (8.40, 28.22, and 88.04 μg/mL). Combining the results of proteomic analysis and enzyme activity assay allows the antibacterial mechanism of V40 to be preliminarily revealed, suggesting its potential as a versatile bactericide in combating bacterial pests in the future.

J Chem Inf Model (impact factor: 5.6) 2 区

dMXP: A De Novo Small-Molecule 3D Structure Predictor with Graph Attention Networks.

Ai, Wu, Zhou, et. al

Abstract:

Generating the three-dimensional (3D) structure of small molecules is crucial in both structure- and ligand-based drug design. Structure-based drug design needs bioactive

conformations of compounds for lead identification and optimization. Ligand-based drug design techniques, such as 3D shape similarity search, 3D pharmacophore model, 3D-QSAR, etc., all require high-quality small-molecule ligand conformations to obtain reliable results. Although predicting a small molecular bioactive conformer requires information from the receptor, a crystal structure of the molecule is a proper approximation to its bioactive conformer in a specific receptor because the binding pose of a small molecule in its receptor's binding pockets should be energetically close to the crystal structures. This study presents a de novo small molecular structure predictor (dMXP) with graph attention networks based on crystal data derived from the Cambridge Structural Database (CSD) combined with molecular electrostatic information calculated by density-functional theory (DFT). Two featuring strategies (topological and atomic partial change features) were employed to explore the relation between these features and the 3D crystal structure of a small molecule. These features were then assembled to construct the holistic 3D crystal structure of a molecule. Molecular graphs were encoded using a graph attention mechanism to deal with the issues of the inconsistencies of local substructures contributing to the entire molecular structure. The root-mean-square deviation (RMSDs) of approximately 80% dMXP predicted structures and the native binding poses within receptors are less than 2.0 Å.

APPLIED PARTIAL DIFFERENTIAL EQUATIONS

IEEE Trans Med Imaging (impact factor: 10.6) 1 区

Magnetic Resonance Electrical Properties Tomography Based on Modified Physics-Informed Neural Network and Multiconstraints.

Ruan, Wang, et. al

Abstract

This paper presents a novel method based on leveraging physics-informed neural networks for magnetic resonance electrical property tomography (MREPT). MREPT is a noninvasive technique that can retrieve the spatial distribution of electrical properties (EPs) of scanned tissues from measured transmit radiofrequency (RF) in magnetic resonance imaging (MRI) systems. The reconstruction of EP values in MREPT is achieved by solving a partial differential equation derived from Maxwell's equations that lacks a direct solution. Most conventional MREPT methods suffer from artifacts caused by the invalidation of the assumption applied for simplification of the problem and numerical errors caused by numerical differentiation. Existing deep learning-based (DL-based) MREPT methods comprise data-driven methods that need to collect massive datasets for training or model-driven methods that are only

validated in trivial cases. Hence we proposed a model-driven method that learns mapping from a measured RF, its spatial gradient and Laplacian to EPs using fully connected networks (FCNNs). The spatial gradient of EP can be computed through the automatic differentiation of FCNNs and the chain rule. FCNNs are optimized using the residual of the central physical equation of convection-reaction MREPT as the loss function (L). To alleviate the ill condition of the problem, we added multiconstraints, including the similarity constraint between permittivity and conductivity and the ℓ1 norm of spatial gradients of permittivity and conductivity, to the L. We demonstrate the proposed method with a three-dimensional realistic head model, a digital phantom simulation, and a practical phantom experiment at a 9.4T animal MRI system.

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

Finite-Time Consensus Adaptive Neural Network Control for Nonlinear Multiagent Systems Under PDE Models.

Liu, Shang, et. al

Abstract

In this article, a novel adaptive control method based on neural networks is proposed for a class of multiagent systems (MASs) with nonlinear functions and external disturbances. First, the approximation properties of neural networks are used to approximate the MAS partial differential equation (PDE) model with nonlinear terms containing two variables, time t, and spatial variable x. Second, an adaptive controller is constructed to actuate the parabolic MAS to reach consensus under external disturbances. Based on this, the finite-time theorem and special inequalities are applied to prove the stability of the closed-loop system. Thus, MAS that have nonlinear functions and external disturbances are enabled with finite-time consensus. Finally, the effectiveness of the proposed control method is demonstrated by numerical simulations.

Neural Netw (impact factor: 7.8) 1 区

Applying Convolutional Neural Networks to data on unstructured meshes with space-filling curves.

Heaney, Li, et. al

Abstract

This paper presents the first classical Convolutional Neural Network (CNN) that can be applied directly to data from unstructured finite element meshes or control volume grids. CNNs have been hugely influential in the areas of image classification and image compression, both of which typically deal with data on structured grids. Unstructured meshes are frequently used to solve partial differential equations and are particularly suitable for problems that require the mesh to conform to complex geometries or for problems that require variable mesh resolution. Central to our approach are space-filling curves, which traverse the nodes or cells of a mesh tracing out a path that is as short as possible (in terms of numbers of edges) and that visits each node or cell exactly once. The space-filling curves (SFCs) are used to find an ordering of the nodes or cells that can transform multi-dimensional solutions on unstructured meshes into a one-dimensional (1D) representation, to which 1D convolutional layers can then be applied. Although developed in two dimensions, the approach is applicable to higher dimensional problems. To demonstrate the approach, the network we choose is a convolutional autoencoder (CAE), although other types of CNN could be used. The approach is tested by applying CAEs to data sets that have been reordered with a space-filling curve. Sparse layers are used at the input and output of the autoencoder, and the use of multiple SFCs is explored. We compare the accuracy of the SFC-based CAE with that of a classical CAE applied to two idealised problems on structured meshes, and then apply the approach to solutions of flow past a cylinder obtained using the finite-element method and an unstructured mesh.

NONLINEAR STABILITY THEORY

IEEE Trans Cybern (impact factor: 11.8) 1 区 TOP

A Modular Event-Triggered Containment Control Scheme for Nonlinear Heterogeneous Multiagent Systems With Unknown Leaders.

Wang, Deng, et. al

Abstract

This article addresses the containment control problem in multiagent systems with nonlinear heterogeneous followers and multiple unknown leaders whose dynamics are exclusively known to their neighbors. The primary goal is to ensure the convergence of each follower to the dynamic convex hull spanned by the leaders under the constraints of limited communication resources. To achieve this, this article introduces a modular event-triggered containment control scheme with three modules. The first module, Module I-signal generator, is designed for each follower to generate a reference signal asymptotically entering the dynamic convex hull without relying on follower dynamics. The second module, Module II-event-triggered mechanism, is tailored to save communication resources effectively by determining when to broadcast information based on perturbed system stability and input-to-state stability theories. The third module, Module III-tracking controller, treats each follower as an independent agent and is crafted to track the reference signal generated by Module I using an output regulation approach. It is established that the system achieves containment control

without Zeno behavior under the influence of these modules, and the theoretical results are validated through simulation examples, demonstrating the practical validity of the proposed approach.

Nano Lett (impact factor: 10.8) 1 区 TOP

Artificial Domain Patterning in Ultrathin Ferroelectric Films via Modifying the Surface Electrostatic Boundary Conditions.

Li, Liao, Deng, et. al

Abstract:

Nanoscale spatially controlled modulation of the properties of ferroelectrics via artificial domain pattering is crucial to their emerging optoelectronics applications. New patterning strategies to achieve high precision and efficiency and to link the resultant domain structures with device functionalities are being sought. Here, we present an epitaxial heterostructure of SrRuO3/PbTiO3/SrRuO3, wherein the domain configuration is delicately determined by the charge screening conditions in the SrRuO3 layer and the substrate strains. Chemical etching of the top SrRuO3 layer leads to a transition from in-plane a domains to out-of-plane c domains, accompanied by a giant (>105) modification in the second harmonic generation response. The modulation effect, coupled with the plasmonic resonance effect from SrRuO3, enables a highly flexible design of nonlinear optical devices, as demonstrated by a simulated split-ring resonator metasurface. This domain patterning strategy may be extended to more thin-film ferroelectric systems with domain stabilities amenable to electrostatic boundary conditions.

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

Adaptive Neural Consensus Observer Networks Design for a Class of Semilinear Parabolic PDE Systems.

Cai, Yuan, et. al

Abstract:

This article concerns the investigation on the consensus problem for the joint state-uncertainty estimation of a class of parabolic partial differential equation (PDE) systems with parametric and nonparametric uncertainties. We propose a two-layer network consisting of informed and uninformed boundary observers where novel adaptation laws are developed for the identification of uncertainties. Particularly, all observer agents in the network transmit their information with each other across the entire network. The proposed adaptation laws include a penalty term of the mismatch between the parameter estimates generated by the other observer agents. Moreover, for the nonparametric uncertainties, radial basis function (RBF) neural networks are

employed for the universal approximation of unknown nonlinear functions. Given the persistently exciting condition, it is shown that the proposed network of adaptive observers can achieve exponential joint state-uncertainty estimation in the presence of parametric uncertainties and ultimate bounded estimation in the presence of nonparametric uncertainties based on the Lyapunov stability theory. The effects of the proposed consensus method are demonstrated through a typical reaction-diffusion system example, which implies convincing numerical findings.

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Ⅱ Concentration

PHYSICS

Realization of an atomic quantum Hall system in four dimensions

Jean-Baptiste Bouhiron, Aurélien Fabre, et al.

Abstract

Modern condensed matter physics relies on the concept of topology to classify matter, from quantum Hall systems to topological insulators. Engineered systems, benefiting from synthetic dimensions, can potentially give access to topological states predicted in dimensions D > 3. We report the realization of an atomic quantum Hall system evolving in four dimensions (4D), with two spatial dimensions and two synthetic ones encoded in the large spin of dysprosium atoms. We measure the nontrivial topological index of the ground band through a full characterization of the nonlinear electromagnetic response and observe the associated anisotropic hyperedge modes. We also excite nonplanar cyclotron motion, in contrast to the planar orbits in D ⩽ 3. Our work may enable the investigation of strongly correlated topological liquids in 4D, generalizing fractional quantum Hall states.

Large-scale photonic chiplet Taichi empowers 160-TOPS/W artificial general intelligence

Zhihao Xu, Tiankuang Zhou, et al.

Abstract

The pursuit of artificial general intelligence (AGI) continuously demands higher computing performance. Despite the superior processing speed and efficiency of integrated photonic circuits, their capacity and scalability are restricted by unavoidable errors, such that only simple tasks and shallow models are realized. To support modern AGIs, we designed Taichi—large-scale photonic chiplets based on an integrated diffractive-interference hybrid design and a general distributed computing architecture that has millions-of-neurons capability with 160–tera-operations per second per watt (TOPS/W) energy efficiency. Taichi experimentally achieved on-chip 1000-category–level classification (testing at 91.89% accuracy in the 1623-category Omniglot dataset) and high-fidelity artificial intelligence–generated content with up to two orders of magnitude of improvement in efficiency. Taichi paves the way for large-scale photonic computing and advanced tasks, further exploiting the flexibility and potential of photonics for modern AGI.

A magnetic massive star has experienced a stellar merger

A. J. Frost, H. Sana, et al.

Abstract

Massive stars (those ⩾8 solar masses at formation) have radiative envelopes that cannot sustain a dynamo, the mechanism that produces magnetic fields in lower-mass stars. Despite this, approximately 7% of massive stars have observed magnetic fields, the origin of which is debated. We used multi-epoch interferometric and spectroscopic observations to characterize HD 148937, a binary system of two massive stars. We found that only one star is magnetic and that it appears younger than its companion. The system properties and a surrounding bipolar nebula can be reproduced with a model in which two stars merged (in a previous triple system) to produce the magnetic massive star. Our results provide observational evidence that magnetic fields form in at least some massive stars through stellar mergers.

MATERIALS

Closed-loop recyclability of a biomass-derived epoxy-amine thermoset by methanolysis

Xianyuan Wu, Peter Hartmann, et al.

Abstract

Epoxy resin thermosets (ERTs) are an important class of polymeric materials. However, owing to their highly cross-linked nature, they suffer from poor recyclability, which contributes to an unacceptable level of environmental pollution. There is a clear need for the design of inherently recyclable ERTs that are based on renewable resources. We present the synthesis and closed-loop recycling of a fully lignocellulose-derivable epoxy resin (DGF/MBCA), prepared from dimethyl ester of 2,5-furandicarboxylic acid (DMFD), 4,4′-methylenebis(cyclohexylamine) (MBCA), and glycidol, which displays excellent thermomechanical properties (a glass transition temperature of 170°C, and a storage modulus at 25°C of 1.2 gigapascals). Notably, the material undergoes methanolysis in the absence of any catalyst, regenerating 90% of the original DMFD. The diamine MBCA and glycidol can subsequently be reformed by acetolysis. Application and recycling of DGF/MBCA in glass and plant fiber composites are demonstrated.

Ultrahigh energy storage in high-entropy ceramic capacitors with polymorphic relaxor phase

Min Zhang, Shun Lan, et al.

Abstract

Ultrahigh–power-density multilayer ceramic capacitors (MLCCs) are critical components in electrical and electronic systems. However, the realization of a high energy density combined with a high efficiency is a major challenge for practical applications. We propose a high-entropy design in barium titanate (BaTiO3)–based lead-free MLCCs with polymorphic relaxor phase. This strategy effectively minimizes hysteresis loss by lowering the domain-switching barriers and enhances the breakdown strength by the high atomic disorder with lattice distortion and grain refining. Benefiting from the synergistic effects, we achieved a high energy density of 20.8 joules per cubic centimeter with an ultrahigh efficiency of 97.5% in the MLCCs. This approach should be universally applicable to designing high-performance dielectrics for energy storage and other related functionalities.

Improved charge extraction in inverted perovskite solar cells with dual-site-binding ligands

Hao Chen, Cheng Liu, et al.

Abstract

Inverted (pin) perovskite solar cells (PSCs) afford improved operating stability in comparison to their nip counterparts but have lagged in power conversion efficiency (PCE). The energetic losses responsible for this PCE deficit in pin PSCs occur primarily at the interfaces between the perovskite and the charge-transport layers. Additive and surface treatments that use passivating ligands usually bind to a single active binding site: This dense packing of electrically resistive passivants perpendicular to the surface may limit the fill factor in pin PSCs. We identified ligands that bind two neighboring lead(II) ion (Pb2+) defect sites in a planar ligand orientation on the perovskite. We fabricated pin PSCs and report a certified quasi–steady state PCE of 26.15 and 24.74% for 0.05– and 1.04–square centimeter illuminated areas, respectively. The devices retain 95% of their initial PCE after 1200 hours of continuous 1 sun maximum power point operation at 65°C.

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Thin adhesive oil films lead to anomalously stable mixtures of water in oil

Claire Nannette, Jean Baudry, et. al

Abstract

Oil and water can only be mixed by dispersing droplets of one fluid in the other. When two droplets approach one another, the thin film that separates them invariably becomes unstable, causing the droplets to coalesce. The only known way to avoid this instability is through addition of a third component, typically a surfactant, which stabilizes the thin film at its equilibrium thickness. We report the observation that a thin fluid film of oil separating two water droplets can lead to an adhesive interaction between the droplets. Moreover, this interaction prevents their coalescence over timescales of several weeks, without the use of any surfactant or solvent.

Force-controlled release of small molecules with a rotaxane actuator

Chen, Lei, et. al

Abstract

Force-controlled release of small molecules offers great promise for the delivery of drugs and the release of healing or reporting agents in a medical or materials context[1,2,3]. In polymer mechanochemistry, polymers are used as actuators to stretch mechanosensitive molecules (mechanophores)[4]. This technique has enabled the release of molecular cargo by rearrangement, as a direct[5,6] or indirect[7,8,9,10] consequence of bond scission in a mechanophore, or by dissociation of cage[11], supramolecular[12] or metal complexes[13,14], and even by 'flex activation'[15,16]. However, the systems described so far are limited in the diversity and/or quantity of the molecules released per stretching event[1,2]. This is due to the difficulty in iteratively activating scissile mechanophores, as the actuating polymers will dissociate after the first activation. Physical encapsulation strategies can be used to deliver a larger cargo load, but these are often subject to non-specific (that is, non-mechanical) release[3]. Here we show that a rotaxane (an interlocked molecule in which a macrocycle is trapped on a stoppered axle) acts as an efficient actuator to trigger the release of cargo molecules appended to its axle. The release of up to five cargo molecules per rotaxane actuator was demonstrated in solution, by ultrasonication, and in bulk, by compression, achieving a release efficiency of up to 71% and 30%, respectively, which places this rotaxane device among the most efficient release systems achieved so far[1]. We also demonstrate the release of three representative functional molecules (a drug, a fluorescent tag and an organocatalyst), and we anticipate that a large variety of cargo molecules could be released with this device. This rotaxane actuator provides a versatile platform for

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various force-controlled release applications.

Couple-close construction of polycyclic rings from diradicals

Long, Alice, et. al

Abstract

Heteroarenes are ubiquitous motifs in bioactive molecules, conferring favourable physical properties when compared to their arene counterparts1,2,3. In particular, semisaturated heteroarenes possess attractive solubility properties and a higher fraction of sp3 carbons, which can improve binding affinity and specificity. However, these desirable structures remain rare owing to limitations in current synthetic methods4,5,6. Indeed, semisaturated heterocycles are laboriously prepared by means of non-modular fit-for-purpose syntheses, which decrease throughput, limit chemical diversity and preclude their inclusion in many hit-to-lead campaigns7,8,9,10. Herein, we describe a more intuitive and modular couple-close approach to build semisaturated ring systems from dual radical precursors. This platform merges metallaphotoredox C(sp2)–C(sp3) cross-coupling with intramolecular Minisci-type radical cyclization to fuse abundant heteroaryl halides with simple bifunctional feedstocks, which serve as the diradical synthons, to rapidly assemble a variety of spirocyclic, bridged and substituted saturated ring types that would be extremely difficult to make by conventional methods. The broad availability of the requisite feedstock materials allows sampling of regions of underexplored chemical space. Reagent-controlled radical generation leads to a highly regioselective and stereospecific annulation that can be used for the late-stage functionalization of pharmaceutical scaffolds, replacing lengthy de novo syntheses.

BIOLOGY

Sexual dimorphism in skin immunity is mediated by an androgen-ILC2-dendritic cell axis

Liang Chi, Can Liu, et al.

Abstract

Males and females exhibit profound differences in immune responses and disease susceptibility. However, the factors responsible for sex differences in tissue immunity remain poorly understood. Here, we uncovered a dominant role for type 2 innate lymphoid cells (ILC2s) in shaping sexual immune dimorphism within the skin.

Mechanistically, negative regulation of ILC2s by androgens leads to a reduction in dendritic cell accumulation and activation in males, along with reduced tissue immunity. Collectively, our results reveal a role for the androgen-ILC2-dendritic cell axis in controlling sexual immune dimorphism. Moreover, this work proposes that tissue immune set points are defined by the dual action of sex hormones and the microbiota, with sex hormones controlling the strength of local immunity and microbiota calibrating its tone.

Molecular mechanism of actin filament elongation by formins

Wout Oosterheert, Micaela Boiero Sanders, et. al

Abstract

Formins control the assembly of actin filaments (F-actin) that drive cell morphogenesis and motility in eukaryotes. However, their molecular interaction with F-actin and their mechanism of action remain unclear. In this work, we present high-resolution cryo–electron microscopy structures of F-actin barbed ends bound by three distinct formins, revealing a common asymmetric formin conformation imposed by the filament. Formation of new intersubunit contacts during actin polymerization sterically displaces formin and triggers its translocation. This “undock-and-lock” mechanism explains how actin-filament growth is coordinated with formin movement. Filament elongation speeds are controlled by the positioning and stability of actin-formin interfaces, which distinguish fast and slow formins. Furthermore, we provide a structure of the actin-formin-profilin ring complex, which resolves how profilin is rapidly released from the barbed end during filament elongation.

Two inhibitory neuronal classes govern acquisition and recall of spinal sensorimotor adaptation

Simon Lavaud, Charlotte Bichara, et. al

Abstract

Spinal circuits are central to movement adaptation, yet the mechanisms within the spinal cord responsible for acquiring and retaining behavior upon experience remain unclear. Using a simple conditioning paradigm, we found that dorsal inhibitory neurons are indispensable for adapting protective limb-withdrawal behavior by regulating the transmission of a specific set of somatosensory information to enhance the saliency of conditioning cues associated with limb position. By contrast, maintaining previously acquired motor adaptation required the ventral inhibitory Renshaw cells. Manipulating Renshaw cells does not affect the adaptation itself but

flexibly alters the expression of adaptive behavior. These findings identify a circuit basis involving two distinct populations of spinal inhibitory neurons, which enables lasting sensorimotor adaptation independently from the brain.

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Ⅲ Calling for papers

AMA 2024

Submission deadline: **Apr 27, 2024**
Conference date: **May 11, 2024 - May 12, 2024**
Full name: **8th International Conference on Applied Mathematics and Sciences**
Location: **Virtual Conference**
Website: https://ama2024.org/

8thInternational Conference on Applied Mathematics and Sciences (AMA 2024)will provide an excellent international forum for sharing knowledge and results in theory, methodology and applications impacts and challenges of Mathematics and Sciences. The conference documents practical and theoretical results which make a fundamental contribution for the development of Mathematics and Sciences. The aim of the conference is to provide a platform to the researchers and practitioners from both academia as well as industry to meet and share cutting-edge development in the field. The goal of this Conference is to bring together researchers and practitioners from academia and industry to focus on Mathematics and Sciences advancements, and establishing new collaborations in these areas. Original research papers, state-of-the-art reviews are invited for publication in all areas of Mathematics.

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:

Advances of Aero space Technology
Abstract Algebra and Applications
Adaptive Control
Agriculture, Environment, Health Applications
Algorithms
Applications of Modelling in Science and Engineering
Artificial Neural Networks (ANN)
Computational Complexity
Computer Modelling
Control Theory
Differential Geometry
Digital Control
Discrete Mathematics
Embedded Systems
Evolutionary Algorithms
Fault Detection and Isolation
Feedback Control
Functional Analysis
Fuzzy logic and Applications
Fuzzy Set Theory
Genetic Algorithms
Genetic Algorithms and Evolutionary Computing
Graph Theory and Applications
Hybrid Systems
Industry, Military, Space Applications
Linear and Nonlinear Control Systems
Linear and Nonlinear Programming
Markov Chains and Applications
Mathematical Modelling
Model Predictive Control
Networked Control Systems Neural
Networks and Fuzzy logic
Neuro-Fuzzy Control
Numerical Analysis

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Numerical Analysis and Scientific Computing
Operations Research
Optimal Control
Optimization and Optimal Control
Optimization Theory
Ordinary and Partial Differential Equations
Process Control and Instrumentation
Real and Complex Analysis
Real-time Issues
Robust Control
Scientific computing
Set Theory
Sliding Mode Control
Soft Computing and Control
Statistics
Stochastic Control and Filtering
Stochastic Modelling
System Identification and Control
Systems and Automation
Topology and Analysis

MATHSJ 2024

Submission deadline: **Apr 28, 2024**
Conference date: **N/A**
Full name: **Applied Mathematics and Sciences: An International Journal**
Location: **N/A**
Website: https://airccse.com/mathsj/index.html

Applied Mathematics and Sciences: An International Journal (MathSJ) aims to publish original research papers and survey articles on all areas of pure mathematics, theoretical applied mathematics, mathematical physics, theoretical mechanics, probability and mathematical statistics, and theoretical biology. All articles are fully refereed and are judged by their contribution to advancing the state of the science of mathematics.

Topics of Interest :

Adaptive control
Agriculture, environment, health applications
Algorithms
Applications of modelling in science and engineering
Artificial Neural Networks (ANN)
Computational Complexity
Computer modelling
Control theory
Differential Geometry
Digital control
Discrete Mathematics
Embedded systems
Evolutionary algorithms
Fault detection and isolation
Feedback control
Functional Analysis
Fuzzy logic and applications
Fuzzy set theory
Genetic Algorithms
Genetic algorithms and evolutionary computing

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Graph Theory and Applications
Hybrid systems
Industry, military, space applications
Linear and nonlinear control systems
Linear and Nonlinear Programming
Markov Chains and Applications
Mathematical modelling
Model predictive control
Networked control systems
Neural networks and fuzzy logic
Neuro-Fuzzy Control
Numerical Analysis
Numerical analysis and scientific computing
Operations Research
Optimal Control
Optimization and optimal control
Optimization Theory
Ordinary and Partial Differential Equations
Process control and instrumentation
Real and Complex Analysis
Real-time issues
Robust control
Scientific computing
Set Theory
Sliding mode control
Soft computing and control
Statistics
Stochastic control and filtering
Stochastic Modelling
System identification and control
Systems and automation
Topology and Analysis

CCCAI 2024

Submission deadline: **Apr 5, 2024**
Conference date: **Aug 23, 2024 - Aug 25, 2024**
Full name: **2024 2nd International Conference on Communications, Computing and Artificial Intelligence**
Location: **Munich, Germany**
Website: http://www.cccai.net/

2024 2nd International Conference on Communications, Computing and Artificial Intelligence (CCCAI 2024) will be held in Jeju, Korea during June 21-23, 2024.
CCCAI is an annual conference which explores the development and implications in the related fields of Communications, Computing and Artificial Intelligence with an objective to present the novel and fundamental advancements. It also serves to foster communication among researchers and practitioners working in a wide variety of scientific areas with a common interest in improving Communications, Computing and Artificial Intelligence. Featured with invited speeches and paper presentations, CCCAI 2024 sincerely welcome interested researchers and professors to understand the frontier research trends and share latest research results, summarize current work and inspire scientific research ideas, broaden horizons and cultivate scientific research interest.

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Call for Papers:
Wireless Communications
Mobile Communications
Information & Communication
Optical Communications
Communication Software
New Communication Technologies
Pattern Recognition
Computer vision
Machine vision
Face recognition
Smart search
Automatic programming
Intelligent and knowledge based system
Visual information processing
(For more topics: http://www.cccai.net/cfp.html)

ICPAM 2024

Submission deadline:	**May 5, 2024**
Conference date:	**Jul 17, 2024 - Jul 20, 2024**
Full name:	**13th International Conference on Pure and Applied Mathematics**
Location:	**Zagreb, Croatia**
Website:	http://www.icpam.org

Conference Summary:
* The 13th International Conference on Pure and Applied Mathematics (ICPAM) will be held in Zagreb, Croatia, July 17-20, 2024. ICPAM is an annual conference that has been successfully organized for ten consecutive years and brings together professors, researchers, scholars, and students in the field of Pure and Applied Mathematics to provide a perfect platform for cross-industry exchanges, sharing of experiences, collaborations among academics, and evaluation of emerging technologies around the world.
* This conference is co-organized by SCIEI, Université d'Orléans, France and Manisa University, Turkey. It is joint supported by Tobb Etu University of Economics and Technology,Turkey; Institute for Economics and Peace; Loughborough University, England; Eskişehir University, Turkey; Southern Federal University, Russia and Academic Network.

***Call for papers:**
* Applied Partial Differential Equations

* Applied Mathematics
* Mathematical Chemistry
* Computational Physics
* Mathematical Biology
* Information Fusion
* Integral Equations
* Mathematical Economics

For more information on the call for papers topics, please go to the official conference website: http://www.icpam.org/scope.html

ICMC 2024

Submission deadline:	**Aug 22, 2024**
Conference date:	**Jan 2, 2024 - Jan 7, 2024**
Full name:	**International Conference on Mathematics and Computing**
Location:	**India**
Website:	http://icmc2024.kalasalingam.ac.in/

Greetings!

Please accept our apologies if you receive multiple copies of this CFP.

Welcome to the 10th International Conference on Mathematics and Computing (ICMC 2024) (http://icmc2024.kalasalingam.ac.in/).

We request you to forward this message to your research group/friends/ colleagues/research students those who are interested.

International Conference on Mathematics and Computing (ICMC) is a premier forum for the presentation of new advances and research results in the field of Cryptology, Network Security, Cybersecurity, Blockchain, IoT, Mobile Network, Data Analytics, Mathematics, Statistics and Scientific Computing etc.

The conference will bring together leading academic scientists, experts from industry, and researchers in their domains of expertise from around the world.

Topics of interest

Computing:

Cryptology and Cyber Security

Network Security

Digital Image Processing
Digital Watermarking
Wireless Networks
Mobile, Distributed, and Parallel Computing
Internet of Things
Machine and Deep Learning
Green Computing
Big Data
Blockchain
Cloud, Fog, and Edge Computing

Mathematics:

Numerical Analysis
Approximation Theory
Analysis
Linear Algebra
Computational Number Theory
Differential Equations
Operations Research
Probability and Statistics
Computational Fluid Mechanics
Mathematical Modeling and Simulation
Applications of Fuzzy Set Theory
Discrete Mathematics
Game Theory
Geometry (Discrete, Algebraic, Finite)
Information Theory

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