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Poster location	Name	Topic	Title	Author(s)	Abstract
19	Zeeshan Ahmad	Physical Science and Engineering	Data-driven Computational Screening of Stable Solid Ion Conductors for Li Metal Anode-based Batteries	Zeeshan Ahmad, Venkat Viswanathan	Li metal is the ideal anode material for batteries due to its high energy density. However, uneven deposition of Li ions during charging causes growth of dendrites which leads to shorting and loss of capacity. Solid electrolytes have been suggested as possible candidates for mechanical suppression of dendrites at the Li metal anode. In this work, we apply statistical learning techniques to predict the mechanical properties of candidate solid electrolytes using structural features of the crystal lattice of the materials as descriptors. The learning is done using the density functional theory predicted mechanical properties of about 250 solid electrolytes. The statistical learning model provides an efficient way to circumvent the challenges associated with high computational costs, while retaining a reasonable accuracy.
20	Joseph Albro	Physical Science and Engineering	Remote and Automatic Data Analysis	Joseph Albro; Jeremy Levy, PhD	An approach to data analysis that allows researchers to view the results of an experiment remotely and in real time.
79	Justin Arnett, MTM	Translational Life Science	Clinical and Surgical Practices and Outcomes for Invasive Brain-Computer Interface Research	Justin Arnett, MTM; Jennifer Collinger, PhD; Michael Boninger, MD; Elizabeth Tyler-Kabara, MD, PhD	There currently exists no literature describing detailed clinical and surgical processes and techniques necessary for invasive human Brain-Computer Interface (BCI) research. Here, we describe processes for subject selection and enrollment, surgical implantation, explantation, and revision of electrodes, postoperative management, and our postoperative results and complications that had yielded successful BCI prosthetic control in all five of our subjects. From 2011 to present, our group implanted electrodes for the purposes of BCI testing in five subjects with complete loss of upper extremity function. Medical chart and study protocol review was conducted to enumerate the processes and results of the research activities noted above. All five subjects demonstrated significant sensorimotor cortex activation in response to attempted movement of their paralyzed upper extremity. All surgical procedures were uncomplicated, without postoperative findings of substantial brain injury. Electrode implantation was correctly targeted in all but two subjects- one in which stable, successful BCI control was still maintained. Microelectrode array pedestal site skin retraction was observed in 2/6 total pedestal sites. Implanted arrays demonstrated stable recording performance in most electrodes throughout their implantation periods. All subjects demonstrated successful BCI performance. This description of our methodology and findings may standardize such practices within the BCI field.
80	Brittany Atuahene	Translational Life Science	The Role of Total Sleep Time in Teen Suicidality	Brittany N. Atuahene, BA; Tina R. Goldstein, PhD	Background: Youth suicide is a significant public health problem. Previous studies have examined the relationship between total sleep time (TST) and suicidal behaviors in adolescents. We hypothesized that both short and long TSTs would be associated with suicidal ideation, attempts, and non-suicidal self-injury (NSSI) in adolescents. Methods: We used logistic regression to evaluate the association between TST and suicidal ideation, attempts, and NSSI over one year in 1,813 adolescents who completed self-report measures as part of the Healthy Allegheny Teens Survey (HATS). Results: We found self-reported suicidal ideation, attempts and NSSI were all significantly associated with both short and long TSTs. Conclusions: Data indicate both short and long TSTs are associated with suicidal ideation, attempts, and NSSI in a community sample of adolescents. TST should be considered in adolescent suicide risk assessment.
21	Jonathan Beaumariage	Physical Science and Engineering	Measurement of Upper Polariton Through PLE	Jonathan Beaumariage	With the development of long life time microcavity quantum well samples, we have lost the ability to directly observe the upper polariton branch. However, by scanning our pump laser's wavelength and observing the lower polariton's intensity, we can determine the upper polariton's wavelength. The major difficulty in doing this is the speed of data collection and finding methods to cut out the reflected laser light from our source.

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1	Alyssa Bell	Basic Life Science	Computational and Experimental Modeling of Cytochrome B5 Reductase Dynamics	Alyssa Bell; Adam Straub, PhD; and Patrick Thibodeau, PhD	Recent clinical and animal studies demonstrate that mutations in human cytochrome B5 reductase (CyB5R3) result in an elevated risk of hypertension and cardiac failure. One of these, T117S is prevalent in 23% of the African-American population. We hypothesized that T117S decreases the thermodynamic stability and increases native-state dynamics of CyB5R3. To test this, we utilized a combination of computational and experimental methods to evaluate CyB5R3 structure. Molecular dynamics simulations identified changes in protein dynamics between the WT and mutant proteins. The mutant protein shows an increase in structural dynamics in these simulations. Thermodynamic stability of the purified CyB5R proteins was then assessed with the ThermoFluor Assay. Thermofluor stability measurements showed a destabilization of CyB5R3 with the T117S mutation by about 2ºC, due to early protein unfolding. Since the T117S variant was shown to exhibit altered protein dynamics, small molecule binding might be a potential therapeutic strategy to revert these conformational changes. A small pilot screen was performed using the ThermoFluor Assay to identify molecules that stabilize CyB5R3. Multiple molecules were found to stabilize the mutant protein. These findings suggest that this approach could be further optimized to identify therapeutics to revert the conformational changes associated with the T117S mutation.
2	Yuemin Bian	Basic Life Science	Computational Chemogenomics-Based Targets Identification and Protein Binding Modes Analysis for Cannabidiol	Yuemin Bian, Xibing He, Lirong Wang, Zhiwei Feng, Junmei Wang, Xiang-Qun Xie	The medical use of cannabis received legal status in 29 states, which include the Pennsylvania, across the United States. Investigations into the ingredients inside the marijuana plants, and the evaluation of drugability for individual or combinational components, turns out to be a research focus for both academic institutions and pharmaceutical companies. With both treatment benefits in central nervous system and the peripheral parts of the body, Cannabidiol (CBD) draws public attention. Considering the complexity of targets network construction, specifying therapeutic targets and signaling pathways for CBD is one of the major obstacles. Here we reported our research on using Chemgenomics technologies for generating targets networks for CBD. In-silico modeling and simulation were followed to evaluate the protein-CBD binding modes for representatives of Class A, rhodopsin-like GPCRs. A hydrophobic cavity and backbone hinge model was proposed and tested. Dopamine receptor 2 was further predicted to be a potential target for CBD.
12	Gibran Biswas	New Research Tools and Techniques	Creating an R Shiny Application to Visualize Gene Expression Data	Gibran Biswas; Uma Chandran, PhD	Next generation sequencing (NGS) is revolutionizing gene expression analysis; it is more accurate, can analyze more genes and produce a more detailed profile of gene expression than previous technologies. This includes RNA-Seq: RNA-Seq are methods that use reverse transcription of RNA to obtain cDNA molecules that produce reads that are then read and aligned to obtain gene expression data. However, Next Generation Sequencing has its share of challenges. The primary one is the large amount of complex data that it produces, which requires expertise in bioinformatics and statistics to analyze and interpret. Therefore, it is often difficult for end-users (i.e. the scientists) to analyze their own data. With this project, I aim to make a tool that can create effective visualization methods and allow the user to navigate these visualizations to answer their questions. To do this, I used R Shiny to make a simple application that makes RNA-seq data easier to manipulate. The program was made to analyze how data on a study that analyzed the effect of Dexamethasone (glucocorticoid) and Statin affect the developing mouse cortex. The application takes RNA-Seq data produced by the aligner Salmon and offers multiple methods of filtering and visualizing the data.

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22	Megan Briggeman	Physical Science and Engineering	Probing 1D Superlattices at the LAO/STO Interface	Megan Briggeman, Patrick Irvin, Mengchen Huang, Anthony Tylan-Tyler, Jungwoo Lee, Hyungwoo Lee, Chang-Beom Eom, Jeremy Levy	Complex oxides and other quantum systems exhibit behavior that is currently too complex to be understood using analytic or computational methods. One approach is to use a configurable quantum system in which the Hamiltonian can be mapped onto the system of interest. This approach, known as quantum simulation, requires a rich physical system whose quanta and interactions can be controlled precisely, at the level of single electrons and other degrees of freedom. Here we describe steps toward developing a quantum simulation platform using the complex oxide heterostructure LaAlO3/SrTiO3 by creating quantum systems with features comparable to the mean spacing between electrons. This interface has strong, sign changing, gate-tunable electron-electron interactions that can strongly influence the quantum ground state. We explore the magnetotransport properties of 1-D superlattices, where periodic modulation produces reproducible dispersive features not seen in control structures. The results of these experiments can be compared with effective 1D model Hamiltonians to bridge experiment and theory and enable quantum simulation of more complex systems.
23	Amy Carlson	Physical Science and Engineering	A Simplified Method of Predicting the Convergence of Properties in Titania Slab Models	Amy N. Carlson; Austin Gagliardi; John C. Kern, PhD; Ellen S. Gawalt, PhD; Jeffrey D. Evanseck, PhD	Accurate theoretical description of surface energy and surface properties is critical to proper modelling of catalysis, crystal growth, and adsorption. However, computational modelling of two-dimensionally periodic systems (i.e. slab models), introduces a problem since sufficiently large models must be used such that the two exposed surfaces are decoupled. Calculations on such large models (10+ layers) can be very computationally costly and may become taxing to determine the point at which the energy will converge. Rutile (110) and anatase (101) were chosen as test cases due to the prevalence of theoretical and experimental data on these surfaces. In order to minimize the number of calculations required for accurate prediction and to capture both oscillatory and non-oscillatory behavior, an exponential functional form is proposed and applied to surface energies, surface relaxations, and adsorption energies.
24	Zhongmou Chao	Physical Science and Engineering	Formation/Dissolution of Conductive Silver Filaments through an Ionic Liquid/Polymer Electrolyte Thin Film	Zhongmou Chao; Brian Radka; Susan Fullerton, PhD	Materials with reconfigurable optical properties are potential candidates for applications such as optical cloaking and wearable sensors. One approach to develop these materials is to create and destroy atomic-scale conductive channels in well-defined locations within a polymer film via field-effect. However, this approach requires a balance between fast ion mobility for fast filament formation/dissolution, along with robust mechanical properties for a flexible film with high elastic modulus. Unfortunately, the properties that promote fast ion transport (e.g., polymer mobility in a solid polymer electrolyte) also degrade the mechanical properties. To address this challenge, a UV-crosslinkable polymer is combined with an ionic liquid and a silver salt. The crosslinkable polymer provides mechanical structure, while the ionic liquid serves as a non-volatile plasticizer to increase ion transport. Poly(ethylene glycol) diacrylate (PEGDA) is the crosslinkable polymer, 1-butyl-3-methylimidazolium hexafluoroborate is the ionic liquid, and AgPF6 is the silver salt. By applying an external field to the solid polymer electrolyte, silver filaments can be created and destroyed on demand. Using a conducting AFM tip as one electrode and a silver substrate as the other, automated measurement of hundreds of filament formation/dissolution events are made at predefined locations in a single experimental session.
25	Lu Chen	Physical Science and Engineering	Carrier Mediated Lattice Distortion in CaZrO3/SrTiO3	Lu Chen; Yunzhong Chen, PhD; Jianan Li; Dennis Valbjørn Christensen, PhD; Nini Pryds, PhD; Patrick Irvin, PhD; Jeremy Levy, PhD	Perovskite oxide heterostructures exhibit a wealth of physical properties and are promising alternatives for future nanoelectronics. A hysteretic piezoelectric-like response has been observed in LaAlO3/SrTiO3(LAO/STO) and this electromechanical response can be attributed to carrier mediated lattice distortions, known as Jahn-Teller effects. Unlike LaAlO3, CaZrO3(CZO) has a lattice constant that is larger compared to SrTiO3, which leads to different lattice distortions when the carrier density changes in CZO/STO. Here we demonstrate the study of the piezoelectric-like response of LAO/STO and CZO/STO using a non-local piezoresponse force microscopy(PFM) technique. Both vertical and lateral PFM responses have been compared.

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26	Caleb Clever	Physical Science and Engineering	Effects of Backbone Composition and Integrity on the Molecular Conductance of Nucleic Acid Duplexes	Caleb Clever; Edward Beall; Emil Wierzbinski, PhD; David Waldeck, PhD	Single molecule conductance measurements are used to determine the conductance of nucleic acid duplexes, with the long-term goal of studying redox-active moieties in precise 3D arrangements on nucleic acid scaffolds. Our results show that the conductance of nucleic acids depends strongly on their backbone composition. For example, DNA and PNA (peptide nucleic acid) differ in conductance by 10 to 100 times for the same sequence. Our data show that this difference is maintained for 10-mer and 20-mer duplexes. In addition, we introduce a break, 'nick', into the backbone of the strand and find that the conductance value is largely unaffected; however the conductance histograms are somewhat broader. These findings suggest that supramolecular assemblies of smaller, stitched components would maintain their high conductance in larger nucleic acid structures, but may suffer from increased variability in molecular conductance.
31	Scott Crawford	Physical Science and Engineering	Using Gold Nanoparticle Surface Chemistry to Control Electronic Behavior: Towards Energy Transfer Applications	Scott Crawford; Christopher Andolina, PhD; Marcus Tofanelli, PhD; Ashley M. Smith, PhD; Kathryn A. Johnston; Michael J. Hartmann; Bo Ryoo	Small gold nanoparticles (AuNPs, ~1.4–2.2 nm core diameters) exist at an exciting interface between molecular and metallic electronic structures. These particles have the potential to elucidate fundamental physical principles driving nanoscale phenomena and to be useful in critical applications ranging from catalysis to bioimaging. We demonstrate surface chemistry-dependent photoluminescent properties of aqueous, phosphine-terminated AuNPs (core diameter = 1.7 ± 0.4 nm) after ligand exchange with a variety of sulfur-containing molecules. No emission is observed from these particles prior to ligand exchange, however the introduction of sulfur-containing ligands initiates photoluminescence, with quantum yields approaching 4% for the smallest ligands studied. With correlation between surface chemistry and AuNP emission properties in hand, the rational design of AuNPs for energy transfer applications is demonstrated by using NIR-emitting AuNPs to sensitize ytterbium (Yb) emission. The AuNP-Yb conjugate combines the high-molar absorptivity (= 1.21x103 M-1cm-1) and broad excitation features of AuNPs with the narrow emission properties of the Yb: AuNP-Yb conjugate exhibits a full-width at half maximum of 62 nm with brightness (x) of 1.9x103 M-1cm-1. Mercaptoalkanoic acid ligands of different chain lengths used to systematically control the distance between the AuNP and ytterbium, yielding distance-dependent results are consistent with Dexter energy transfer mechanism.
15	Leyan deBorja	New Research Tools and Techniques	Using Focus Groups to Explore Cultural Acceptability of LARC	Yassmin Al Aaraj, MD, MPH; Leyan deBorja, MPH; John Maier, MD, PhD; Chyongchiou lin, PhD; Jeannette E. South-Paul, MD	Title: Using focus group to explore cultural acceptability of long acting contraception in a diverse, urban population Context: Long-acting reversible contraceptive methods (LARCs) have been found to be highly effective in reducing the incidence of unintended pregnancy. However, rates of LARC usage remain low compared to other contraceptive methods. Objective: To explore cultural acceptability of LARCs in a diverse, urban population. Design: Participants were recruited from seven UPMC affiliated family health centers (FHCs) located in Pittsburgh. Participants were asked to attend a 60 to 90-minutes focus group session. The sessions were directed by a trained facilitator, who engaged participants in a general discussion about contraception and LARCs. Recruitment was conducted through fliers, and by word of mouth from recruited participants. Participants were asked to complete a brief demographic survey. Participants: 7 focus groups, consisting of 7 to 12 women, were conducted. 64 women in total between 18 and 45 years of age, who were not pregnant, were recruited to take part in the focus group sessions. Results: Different themes emerged from the focus group sessions like pressure to utilize birth control, side effects linked to LARCs, male contraception, and information about birth control methods provided by physicians.

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32	Cheng Fang	Physical Science and Engineering	Computational Studies of Copper-Catalyzed and Photoinduced Metal-Free Atom Transfer Radical Polymerization	Cheng Fang, MS; Xiangcheng Pan, PhD; Marco Fantin, PhD; Armando Genaro, PhD; Krzysztof Matyjaszewski, PhD; Peng Liu, PhD	Atom transfer radical polymerization (ATRP) is among the most powerful and robust controlled radical polymerization techniques that facilitates macromolecular engineering by synthesis of polymers with precise molecular weights, low dispersities, and well-controlled architectures. Good control over polymer structures via ATRP is largely attributed to the fast activation/deactivation equilibrium that can be governed by transition metal catalysts (particularly with copper catalysts) or photoredox catalysts. However, the detailed mechanism of ATRP has not been studied thoroughly at the atomic level, which hinders the rational design of better ATRP catalysts. In this study, we employ density functional theory (DFT) and Marcus Theory calculations to investigate both outer-sphere single electron transfer (OSET) and inner-sphere single electron transfer (ISET) pathways for photoinduced ATRP systems with phenothiazine derivatives as photoredox catalyst.
33	Adelle Fernando	Physical Science and Engineering	A Machine Learning Approach to Classifying Acute Pain Using Time Scale Decomposition of EDA Signals	Adelle Fernando; Busra Susam, MS; Murat Akcakaya, PhD	Currently, methods of pain evaluation and diagnosis in the clinical setting are subjective and incoherent. The objective of this project is to classify acute pain in adolescents through the combination of electrodermal activity signals (EDA) and a feature extraction technique called time scale decomposition (TSD) for use in machine learning algorithms. EDA data was used for its connection to the sympathetic nervous system and pain response. Signals were collected from fifteen post-appendectomy patients during three visits, with Visit 1 and Visit 3 representing pain and no pain, respectively. The signal data was then downsampled, filtered, normalized, and converted into TSD matrices for feature extraction. Mean, standard deviation, and entropy were selected as features, and dimensionality reduction was performed on the TSD matrices using k-means clustering. After compiling all patient features, the reduced matrices were used in linear discriminant analysis (LDA), a machine learning classifier, which was able to classify acute pain of the tested patients. To extend this project, other classifiers including quadratic discriminant analysis and support vector machines could be used alongside LDA to provide a more in-depth classification. In the future, this system could be implemented in a clinical setting to diagnose pain with less subjectivity.
34	Xing Yee Gan	Physical Science and Engineering	Correlating Carrier Densities in Plasmonic Copper Selenide with Structure, Composition and Surface Chemistry	Lauren Marbella, PhD; Derrick Kaseman, PhD; Emily Eikey; Paige Moncure; Jill Millstone, PhD	Here, we study carrier density in a well-studied non-noble metal plasmonic system, Cu2-xSe. Using 77Se solid state NMR spin lattice relaxation measurements, we track and quantify carrier density changes as a function of particle oxidation. We find that 77Se NMR spectroscopy is a sensitive technique able to identify and measure carrier density in Cu2-xSe systems that are metallic, but that do not yet show optically discernable plasmonic features. Importantly, 77Se NMR simultaneously provides critical information about the structural evolution of these particles as a function of progressive oxidation. Taken together, we then specifically study surface chemistry dependent LSPR behaviors in these nanoparticles, and decouple the influence of changes in medium dielectric properties from ligand-induced carrier density changes.
3	Madhavi Ganapathiraju, PhD	Basic Life Science	367 Novel Protein-Protein Interactions in Malignant Pleural Mesothelioma Interactome	Kalyani Bindu, BS; Madhavi Ganapathiraju, PhD	Malignant Pleural Mesothelioma (MPM) is an aggressive cancer without an identifiable pre-malignant stage that arises due to long-term exposure to asbestos and results in poor prognosis. Discovering PPIs of BAP1 involved in transcriptional regulation has helped translate research in MPM to drug development in the past. By applying our computational methods for High Confidence Protein-Protein Interaction Prediction (HiPPIP) to 62 MPM associated genes, we predicted 367 novel high confidence PPIs adding to about 1,387 previously known PPIs. The novel PPIs provide clues to MPM etiology. Novel interaction DPYSL2-TUBA4A may reveal that axon guidance molecules in the nervous system also participate in lung development and contribute to MPM. That biosynthetic, DNA damage repair and cell survival pathways converge to allow malignant transformation of pleural cells may be demonstrated by novel interactions of ATIC. Novel interactors of FLT1 and FLT3 embedded in a highly connected module of key players in VEGF signaling, some of which are differentially expressed on exposure to crocidolite fibres, may throw light on induction of angiogenic responses and regulation of endocytic trafficking of receptors contributing to MPM. Mechanisms by which PI3K/AKT signaling becomes aberrantly active in MPM may be revealed by novel interactions of PRR5.

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17	Madhavi Ganapathiraju, PhD	New Research Tools and Techniques	Inviting Scientists to Write, Review, and Vote on Biological Hypotheses Derived from Computationally Predicted Protein-Protein Interactions	Madhavi Ganapathiraju, PhD; Kalyani Bindu, BS	Protein-protein interactions (PPIs) are central to cellular systems. Yet less than 10% of estimated PPIs are known today. To accelerate their discovery, we have computationally predicted PPIs which are deemed accurate, according to computational evaluations and experimental validations. If a philanthropist gave funds to study the 100 most impactful PPIs in lab, which 100 should they be? We created a web resource that allows scientists to post a hypothesis about the importance of any PPI, and other scientists to discuss/vote on them, so that over a course of time, PPIs can be prioritized based on these discussions. To get the opinion on biologists about this approach, we present here some novel PPIs with some proposed hypotheses about their biological relevance. Hypotheses will be presented for novel PPIs that may associate cilia dysfunction in ependymal cells to microcephaly, or those that shed light on mechanisms of host invasion adopted by Zika virus, or PPIs that allude comorbidity of Parkinson's disease and limbic epilepsy with congenital heart disease. We invite scientists to comment on this approach, and to vote on these hypotheses. We will demonstrate a website that facilitates such 'asynchronous' collaborations among scientists.
35	Supriya Ghosh	Physical Science and Engineering	Chirality and Light Polarization Effects on Electron Transfer Rate	Supriya Ghosh; Brian P. Bloom, PhD; David Waldeck; PhD	Electron spin and molecular chirality are emerging as factors that can be used effectively to direct charge flow at the molecular scale. We report order of magnitude effects of molecular chirality on electron-transfer rates between quantum dots (QDs) in chiral QD assemblies. Our experiments show that electron transfer from a QD donor to a chiral QD acceptor strongly depends on the light polarization used to excite the donor QD, as well as the chirality of the acceptor QD. We define an asymmetry parameter for the electron transfer rates with polarization and show that it correlates with the strength of the acceptor QD circular dichroism (CD) spectrum. These findings indicate that the CD strength of the QD exciton transition(s) may be used as a predictor for the spin dependent electron transfer. Current studies are focused on understanding how chirality controls the kinetics of electron transfer within the frame work of Marcus theory and how the bridge chirality in the QD assembly influences the asymmetry in electron transfer rates.
81	Lauren Goldschen	Translational Life Science	Coping with Eating Disorders on a College Campus: A Qualitative Study	Lauren Goldschen; Wynne Lundblad, MD; Alexis M. Fertig, MD, MPH; Judy C. Chang, MD, MPH	Study: Anorexia Nervosa and Bulimia Nervosa are eating disorders that are more prevalent on college campuses than in the general population. It is unknown how students with eating disorders use and perceive these resources. Our study's objective is to understand the experiences of undergraduate students with eating disorders regarding managing their disorder during college, preferences for treatment, and challenges when seeking care. Methods: Undergraduate students who self-identify having an eating disorder were recruited through fliers and Project Heal, the undergraduate eating disorder advocacy organization. We conducted semi-structured individual interviews and two investigators separately coded verbatim transcripts. Results: Sixteen undergraduate students participated in the interviews. Participants reported a combination of restricting, binging, purging, and self-harm behaviors. Preliminary analysis of the transcripts has noted the following themes: 1) participants attributed a negative influence on their recovery to the campus unhealthy diet culture; 2) participants described mental illness stigma on college campuses as a barrier to access treatment; 3) participants emphasized a desire for peer support for students with eating disorders on campus. Conclusion: Our preliminary findings suggest a need to provide campus support to students with eating disorders as well as to pursue efforts to reduce stigma regarding mental illness.

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36	Mitchell Groenenboom	Physical Science and Engineering	Inhibiting Oxygen Reduction Reaction Catalysis with Doped Amorphous Ti Oxides	Mitchell C. Groenenboom; Rachel M. Anderson, PhD; Derek J. Horton, PhD; Yasemin Basdogan; Donald F. Roeper, PhD; Steven A. Policastro, PhD; John A. Keith, PhD	Galvanic junctions between dissimilar metals can expedite the corrosion of the less stable metal. This effect is powerful enough to corrode alloys that are normally stable in isolation. The cathodic reactions that occur on the more noble metal surface can limit the rate of corrosion damage in atmospheric conditions. To decrease the driving force for galvanic corrosion, we use Kohn-Sham density functional theory to predict metal dopants that most inhibit the oxygen reduction reaction on amorphous Ti oxide surfaces. We show that by calculating ORR overpotentials for dopants embedded in an amorphous TiO2 surface model we can successfully predict ORR activity trends for 7 different dopants (Ag, Sn, Cr, Co, Al, Mn, and V). We then show that ORR activity trends do not significantly change when calculated with hybrid DFT (HSE06) and VASPsol continuum solvation.
37	Qing Guo	Physical Science and Engineering	Nanoscale Control of the Charge Neutrality Point of Graphene	Qing Guo,MS; Jianan Li, MS; Shivendra Tripathi, MS; Mengchen Huang, PhD; Jen-Feng Hsu, PhD; Shonali Dhingra, PhD; Hyungwoo Lee, PhD; Sangwoo Ryu, PhD; Chang-Beom Eom, PhD; Brian D'Urso, PhD; Patrick Irvin, PhD; Jeremy Levy, PhD	Nano-engineered graphene devices exhibit controllable electronic and optical properties. The two-dimensional electron gas (2DEG) appearing at the Lanthanum aluminate-strontium titanate (LaAlO3/SrTiO3) interface makes it an ideal substrate to pattern nanostructures on graphene through Conductive atomic force microscopy (c-AFM) lithography. Here we report the high quality graphene growth by atmospheric pressure chemical vapor deposition (APCVD) on ultra-flat diamond turned copper substrates. Then the Graphene is transferred to LAO/STO substrated with an amorphous perfluoropolymer Hyflon AD60. Owing to the high dielectric constant of SrTiO3 in low temperature, it is possible to heavily dope graphene and tune the carrier density dramatically. Thus, LAO3/STO3 makes it possible to tune the fermi level and created nanostructures reversibly on graphene.
38	Shan Hao	Physical Science and Engineering	Tuning Critical Thickness by Capping Nanoscale Al on LAO/STO Surface	Shan Hao; Jeremy Levy; Jianan Arthur Li; Patrick Irvin; Hyungwoo Lee; Jung-Woo Lee; Chang-Beom Eom	The interface of LAO/STO supports a 2D electron gas that can be further patterned into 1D structures using an atomic force microscope. As grown, LAO/STO has a critical thickness of 4 unit cells (uc) of LAO. By capping the surface of LAO/STO with Al, the critical thickness can be reduced from 4 uc to 1 uc. Our aim is to pattern Al, with nanoscale precision, in order to locally control the conductance at the LAO/STO interface. Using various patterns, we will create novel quantum structures in order to perform quantum simulation by creating an artificial Hubbard Hamiltonian. These devices also have the potential to be coupled to other Al-based, superconducting devices such as SQUIDs and superconducting microwave resonators.
39	Michael Hartmann	Physical Science and Engineering	Treating Electronic Near Degeneracies at Mean Field Cost	Michael Hartmann; Daniel Lambrecht, PhD	Accurate computational predictions on molecules with near-degenerate electronic states are essential for understanding and controlling some of the most interesting processes in catalysis and spectroscopy. However, cost-efficient density functional theory approaches can be qualitatively incorrect for energetics of near-degenerate states, whereas highly accurate methods suffer from prohibitive exponential scaling of computational cost. We present the direct energy minimization as a function of the single-particle density (DM1D) approach to accurately treat near-degenerate electronic states at mean-field cost. DM1D assigns orbitals to independent active spaces and determines the optimal energy by distributing electron density via a single variational degree of freedom per active space. This ansatz reduces the computational cost form exponential to linear-scaling with the number of active orbitals. Here we combine our approach with configuration interaction single and doubles to capture both near-degeneracy (static) and dynamic electron correlation (DM1D-CISD). We show that DM1D-CISD systematically increases the amount of electron correlation captured across the N2 potential energy surface, a notoriously difficult benchmark , to approximate MRCISD results with similar active spaces. Further, DM1D-CISD captures multiconfiguration effects in diradical such as twisted ethylene, decreasing errors in relative energies between planar and twisted conformers by 64%.
40	Yuchi He	Physical Science and Engineering	Neuron Network Variational Approaches to Solve Many-body Ground States	Yuchi He, Roger Mong	Neuron network type of wave functions are benchmarked for solving ground states of one dimensional quantum models.

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41	Bryan Henderson	Physical Science and Engineering	Using the Fourier Grid Hamiltonian Method to Investigate the Intermolecular Rock Vibration of NO3-H2O	Bryan Henderson; Kenneth Jordan, PhD; Eric Kratz, PhD	In this work, we investigate the intermolecular rock vibration of the gas phase nitrate-water dimer. This mode is coupled with the water OH stretch mode, causing a progression of observed peaks in experimental spectra. However, this rocking mode is difficult to describe theoretically because it is highly anharmonic and very large in amplitude. Additionally, the shape of the rock potential changes depending on if the OH stretch is in the ground or excited state. To deal with these issues, we have calculated the rock mode using the Fourier Grid Hamiltonian Discrete Variable Representation, factoring in the coordinate dependence of the reduced mass due to the large amplitude of the normal mode. Using this method, we have been able to predict the experimental vibrational spectra much more accurately than previous calculations. These techniques should be readily applicable to other large amplitude normal modes that are difficult to describe with conventional methods.
42	Yang Hu	Physical Science and Engineering	Single-electron Transport in One-dimensional Waveguide at LaAlO3/SrTiO3 Interface	Yang Hu, Dengyu Yang, Yun-Yi Pai, Jianan Arthur Li, Patrick Irvin, Jeremy Levy	It's been experimentally demonstrated that two dimensional electron gas (2DEG) can form at the interface of LaAlO3/SrTiO3 heterostructure. Such LAO/STO heterostructures also exhibit electric-field-induced metal-insulator transition when LAO is about 3 unit cells thick. Therefore, nanowire can be written at the interface using positively biased AFM tip. In this project, we aim to realize controllable single-electron transport which will provide on-demand single-electron source for nanoelectronic applications. Here, we fabricate a 1-D waveguide containing electron reservoir-quantum dot- electron reservoir structure in the LAO/STO interlayer with two side-gates tuning tunnel barriers. Electrons in the quantum dot are strongly localized so that the dot only hold integer number of electrons. Electron tunneling happens when a charge state lies between the electrochemical potentials of the two reservoirs. By applying voltage signal with rf frequency to the side-gates, a quantized current is expected when only integer electrons pass through the quantum dot each rf cycle. The current should depend on the phase shift between the two side-gate signals. We investigate the current's dependence on the phase shift by introducing a tiny frequency difference between the two side-gate signal and the I-t curve shall reveal this dependence.
82	Cecilia Huang	New Research Tools and Techniques	Screening for Intimate Partner Violence at the Initial Obstetric Visit	Cecilia Huang, BS; Judy Chang, MD, MPH	Background: One in four women in the US will experience intimate partner violence (IPV) during her lifetime, and screening by healthcare professionals is recommended at each office visit. This project aims to describe the content and style of provider screening for IPV in the initial obstetric visit and describe the relationship between screening and disclosure of IPV. Methods: We recorded obstetric visit interviews at a hospital-based clinic in Pittsburgh, PA. A total of 248 recordings were transcribed and separately coded in an iterative fashion by two coders. Results: IPV screening occurred in 95% of visits, and 57% of these visits included only direct screening questions. Patients disclosed IPV in 70 (28.2%) visits. Nurse midwives were the clinicians most likely not to screen at visits (6/40, 15%); however, they also had one of the highest patient disclosure rates (14/40, 35%). Certified nurse practitioners always screened but had one of the lowest rates of disclosure at visits (5/26, 19%). Conclusions: There are a variety of questions used to screen for IPV at the initial OB visit. That nurse midwives prompted a greater rate of disclosure despite screening less frequently suggests that another facet of the patient-provider relationship plays a role in disclosure.

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16	Yankang Jing, MS	New Research Tools and Techniques	Deep Learning-Based Prediction of Drug-Target Interaction	Yankang Jing, Lirong Wang, Xiang-Qun (Sean) Xie	In silico prediction of potential drug-target interactions (DTIs) has become a routine process for investigating adverse drug effects and repositioning existing or abandoned drugs in computer-aided drug design. With the explosive growth in number of published chemicals in small molecule drug discovery in the last decade, as well as the rapid development of supercomputing technologies recently, it is necessary and feasibly to develop new computational methods to predict unknown DTIs. As a drug can generally have interactions with multiple biological targets, in silico prediction of DTIs is usually considered as a multiclass classification problem with a great number of classes equal to the number of biological targets. Rather than transforming the multiclass problem into a binary classification problem, by which major of the current methods attained their goals, we proposed a novel scheme using deep learning technology to achieve the idea of personalized recommendation to identify potential DTIs using an adaptive model. The model combines feature embedding in distributed representation and convolutional neural networks (CNNs), both of which are the state-of-the-art techniques in deep learning. Evaluation over our large-scale dataset has been done using 10-folds cross validation.
83	Peter Jones, PhD	Translational Life Science	Cortical Neural Activity during Speech in Patients with Movement Disorders	Peter W Jones, PhD; Witold J Lipski, PhD; Ahmad Alhourani, MD; Tara Pirnia, BS; Christina Dastolfo-Hromack, MS; Donald J Crammond, PhD; R Mark Richardson, MD, PhD	Speech is a complex motor pattern that, like other skeletal movements, becomes disrupted in patients with movement disorders, two of the most common being Parkinson's disease (PD) and essential tremor (ET). Nearly all patients with PD will eventually suffer from speech production deficits, characteristically hypokinetic dysarthria, which can lead to significant communication deficits and social isolation. Essential tremor is a movement disorder with a kinetic tremor as its main classical symptom, with 1/5 of ET patients possessing a vocal tremor. Current medical and surgical treatments for PD/ET speech deficits are not as effective as for other motor symptoms, the underlying reasons for which are unknown. Understanding of how activity in the neural circuitry responsible for speech production is altered in these disorders would potentially allow for new therapies to address these symptoms. To study this, we recorded cortical surface local field potentials (LFPs) and spoken acoustics while 14 PD subjects and 11 ET subjects performed a speech task during awake DBS surgery. On each trial, subjects were asked to read aloud a consonant-vowel-consonant syllable presented on a computer screen. Spectral analysis of cortical LFP responses during speech will be demonstrated and compared between subject groups.
43	Matei Jordache	Physical Science and Engineering	Few-Layer Transition Metal Dichalcogenide Exfoliation, Characterization and Modeling for Future Electronic Devices	Matei Jordache; Jerry Liang; Susan Fullerton, PhD	Transition metal dichalcogenides (TMDs) possess unique electrical and mechanical properties when isolated to thin flakes, making them desired for advanced electronic devices. These devices offer potential advantages over traditional devices, including lower power consumption, smaller size, and larger ON/OFF current ratio. Specifically, molybdenum disulfide (MoS2) and molybdenum ditelluride (MoTe2) are of interest- however, the process for isolating flakes for devices is unpredictable. We found that both reactive ion etching before deposition and annealing before exfoliation will increase flake yield and thinness. The increased yield and quality of flakes obtained with reactive ion etching (RIE) and annealing can be attributed to increasing the flake's contact area with the substrate. After exfoliation, we characterize the lateral size and surface roughness of the flakes using atomic force microscopy (AFM). The ideal flake shape is rectangular, with length from 10-30 µm and width from 2-3 µm. The average surface roughness measured is ~0.4 nm for MoS2 exfoliated using the unmodified method, and the average surface roughness is measured at ~0.4nm for MoS2 exfoliated using the modified method, which proves the new method does not impact flake quality. The devices are also being modeled in COMSOL Multiphysics to provide insight into electrical and mechanical behavior.
45	Paul Justice	Physical Science and Engineering	Developing Robust Sequences of Clicker Questions Using Research-validated Tutorials	Emily Marshman, PhD; Chandralekha Singh, PhD	Effective use of clicker questions in physics courses at all levels and in classes of all sizes can be an excellent formative assessment tool and can help students learn physics and develop their reasoning and meta-cognitive skills. Here we discuss our research on the development and evaluation of effective clicker question sequences for helping students learn quantum mechanics. We also discuss research evaluating an effective balance of peer discussions in small groups vs. general class discussions when students engage with different clicker question sequences.

46	Arailym Kairalapova	Physical Science and Engineering	Nonvalence Correlation-bound Anion States	Arailym Kairalapova; Kenneth Jordan	We study non-valence correlation-bound (NVCB) anions using a (H2O)4 cluster model, comprised of two interacting water dimers. The distance between the two water molecules in each dimer is fixed at 3.461 Å, and the electron binding energy is calculated as a function of inter-dimer distance. For dimer separations greater than 4.5 Å, electrostatic interactions are sufficient to bind the excess electron. At distances smaller than 4.5 Å, electrostatic interactions are inadequate to bind the excess electron, but when combined with dispersion-type correlation interactions, the excess electron is still found to bind. The orbital that binds this electron is very diffuse and has a relatively small weight in the valence region. By definition, dispersion-type correlation interactions are not included in Hartree-Fock (HF) and, therefore, methods that assume that the final charge distribution is close to the HF charge distribution fail to bind the excess electron. We demonstrate that it is essential to employ a method that allows for orbital relaxation in response to correlation effects for describing NCVB anions.
47	Christof Keebaugh	Physical Science and Engineering	Investigating and Addressing Student Difficulties with the Representation in which an Operator is Diagonal in the Context of Degenerate Perturbation Theory	Christof Keebaugh, MS; Emily Marshman, PhD; Chandralekha Singh, PhD	We discuss an investigation of student difficulties with determining the representation in which a Hermitian operator corresponding to a physical observable (e.g., the Hamiltonian operator corresponding to energy) is diagonal in the context of degenerate perturbation theory (DPT) involving the Zeeman effect in the hydrogen atom carried out in advanced quantum mechanics courses by administering free-response and multiple-choice questions and conducting individual interviews with students. We find that students share many common difficulties related to these concepts. We describe how the research on student difficulties was used as a guide to develop and evaluate a Quantum Interactive Learning Tutorial (QuILT) which strives to help students develop a functional understanding of linear algebra concepts in the context of DPT. We discuss the development of the DPT QuILT and its evaluation in the undergraduate and graduate courses focusing on these issues.
84	Spencer Keil	Translational Life Science	Perceived Gun Access and Gun Carrying among Male Adolescent Offenders	Spencer Keil, Carol Schubert, Edward Mulvey, Jordan Beardslee, Dustin Pardini	Objective: To determine whether perceived access to guns has a significant, independent effect on gun carrying after adjusting for other static and time-varying factors related to maturity and social context. Methods: Longitudinal observational cohort study of 900 serious adolescent offenders recruited between 2000-2006. Data were obtained through self-report in interviews conducted every six months for three years. Gun access was measured by a rating of whether or not a young person could buy a gun in their neighborhood. Gun carrying was reported as having carried at least once in the recall period. Results: 319 (35.4%) participants reported carrying a gun at least once during the entire study period and 769 (85.4%) reported being able to purchase a gun at least once during that time. Even after adjusting for individual background, maturity, and contextual variables, perceived gun access was significantly related to concurrent gun carrying (AOR=1.41 [1.03,1.94]) as well as carrying in the subsequent recall period (AOR= 1.52 [1.10,2.11]). Conclusions: Self-reported gun access is a significant factor independently related to gun carrying in high-risk youth. Further research on how gun policy and intervention programs may affect perceived access is warranted to design effective interventions for reducing gun violence.
48	Derek Lau	Physical Science and Engineering	Effect of Seedlayer Alloying on the Dzyaloshinskii-Moriya Interaction in Magnetic Thin Films	Derek K. Lau, MS; James P. Pellegren, PhD; Vincent Sokalski, PhD	The interfacial Dzyaloshinskii-Moriya Interaction (DMI) is a spin-orbit interaction in heavy metal(HM)/ferromagnet(FM) heterostructures, which has attracted significant attention because it stabilizes chiral magnetic features that are promising for next-generation spintronics. While work has been done on exploring pure elements for HM/FM structures, the range of possible alloy combinations remain largely unexplored. The ability to tune DMI via composition without compromising other magnetic properties is critical for engineering future devices. We examine the impact of Pt-Ir and Pt-Au alloying on DMI by studying asymmetric domain growth in Co/Ni multi-layers using Kerr Microscopy. We have fabricated magnetic multilayers with varying HM composition and uniform FM (Co/Ni) structures using combinatorial sputtering techniques. We have observed distincts trends in DMI as a function of composition including a reversal in sign despite relatively small changes to other conventional magnetic properties. In addition, we have developed a model of domain wall motion to explain anomalous trends, which we leverage in this study to disentangle the various factors contributing to DW mobility beyond DMI.

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49	Maxwell Li	Physical Science and Engineering	Examining the Internal Magnetic Domain Wall Structure in Co/Ni Multi-layers by Lorentz TEM	Maxwell Li; Marc De Graef, PhD; Vincent Sokalski, PhD	Topological magnetic features such as Skyrmions and chiral domain walls (DWs) have emerged recently as candidates for future computer memory and logic, in part, due to the unprecedented efficiency with which they can be manipulated by electric current. These features are stabilized by the Dzyaloshinskii-Moriya interaction (DMI), which favors a chiral winding of electron spin vectors and greatly affects DW properties. Knowledge of the internal structure of such DWs has become critical to explaining these properties, which requires high resolution magnetic imaging. Here we examine perpendicularly magnetized Co/Ni thin film multi-layers by experimental Lorentz transmission electron microscopy (TEM) coupled with micromagnetic simulations of the spin configuration. The impact of external magnetic field on the domain structure as well as defects that exist within the DWs were studied. Ex-situ application of an in-plane magnetic field gives rise to a stripe domain pattern while in-situ perpendicular fields lead to the stabilization of magnetic bubble domains. Moreover, a significant density of one-dimensional DW defects called vertical Bloch lines are observed and also found to be strong function of the field history.
50	Jianan Li	Physical Science and Engineering	Method for Transferring High-Mobility CVD-Grown Graphene with Perfluoropolymers	Jianan Li; Jen-Feng Hsu, PhD; Hyungwoo Lee, PhD; Shivendra Tripathi; Qing Guo; Lu Chen; Mengchen Huang, PhD; Shonali Dhingra, PhD; Jung-Woo Lee, PhD; Chang-Beom Eom, PhD; Patrick Irvin, PhD; Jeremy Levy, PhD; Brian D'Urso, PhD	The transfer of graphene grown by chemical vapor deposition (CVD) using amorphous polymers represents a widely implemented method for graphene-based electronic device fabrication. However, the most commonly used polymer, poly(methyl methacrylate) (PMMA), leaves a residue on the graphene that limits the mobility. Here we report a method for graphene transfer and patterning that employs a perfluoropolymer—Hyflon—as a transfer handle and to protect the graphene against contamination from photoresists or other polymers. CVD-grown graphene transferred this way onto LaAlO$_3$/SrTiO$_3$ heterostructures is atomically clean, with high mobility (˜30,000 cm^{2}V$^{−1}$s$^{−1}$) near the Dirac point at 2 K and clear, quantized Hall and magnetoresistance. Local control of the LaAlO$_3$/SrTiO$_3$ interfacial metal-insulator transition—through the graphene—is preserved with this transfer method. The use of perfluoropolymers, such as Hyflon, with CVD-grown graphene and other 2D materials can readily be implemented with other polymers or photoresists.
4	Lifan Liang	Basic Life Science	Integrating Information from Perturbation Data and Topic Modeling to Identify Functional Modules in Protein Interaction Networks	Lifan Liang, Vicky Chen, Xiaonan Fan, Songjian Lu	Background: High-throughput biological experiments provided the opportunity to investigate functional interactions among genes and proteins at the full genomic scale. Numerous insights have been gained from computational analysis of a particular omics platforms. It seems promising to integrate information from multiple platforms to generate novel biological hypothesis with higher confidence. Objective: From a graph theoretic stand point, this study aims to develop a way to identify functional modules based on aggregated networks from multiple clues of functional interactions between genes. Data and Method: High-throughput data and topic gene relations computed from text mining in the species of yeast data were used. High-throughput datasets are protein-protein interactions and microarray expressions. we constructed layers of gene network from each type of these data, and combined these layers into a multiplex network. Clustering methods are conducted on both the multiplex and the single layers. Clustering results were compared across different clustering methods and different network construction networks. Results: Functional modules identified from multiplex are more accurate than single-layer networks despite which clustering method was used. Conclusion: The multiplex approach to integrate multiple data sources to improve computational methods are shown to be effective.

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51	Jierui Liang	Physical Science and Engineering	Electric Double Layer Doping of Two-dimensional Semiconductor FETs Using a Monolayer Electrolyte	Jierui Liang; Ke Xu, PhD; Susan Fullerton, PhD	An electric double layer (EDL) formed at the interface between an electrolyte and a two-dimensional (2D) semiconductor can induce large capacitance densities (1-10 μF/〖cm〗^2) and sheet carrier densities ~〖10〗^14 cm^(-2) in 2D crystal field-effect transistors (FETs). In this study, the EDL doping of MoS2 and WSe2 FETs were achieved using a monolayer electrolyte developed by our group (cobalt crown ether phthalocyanine (CoCrPc) with LiClO4). We demonstrate that under a gate bias, Li+ moves towards the interface through CoCrPc to induce image charges in the channel giving n-type doping. Backgated MoS2 and WSe2 FETs were fabricated and a monolayer of CoCrPc was deposited by drop-casting and annealing. The thickness of the monolayer electrolyte is 5 to 7 Å by Atomic Force Microscopy (AFM). MoS2 FET transfer characteristics after programming showed bistability of the monolayer electrolyte, with the extent of n-type doping depending on the magnitude of the applied bias, and the direction of the doping (more or less n-type) depending on the polarity of the applied bias. The threshold voltage shift corresponds to a sheet carrier density of ~〖10〗^12 cm^(-2). Future efforts will be fabricating top-gate FETs doped by the monolayer electrolyte.
5	Qiao Lin, MPH	Basic Life Science	Lung Microenvironment Determines the Susceptibility to Respiratory *Pseudomonas aeruginosa* Infection	Qiao Lin, Y. Peter Di	Cystic fibrosis (CF) is a genetic disease with a loss of CFTR function that leads to impaired airway host defense. Chronic infection by *Pseudomonas aeruginosa* (*P. aeruginosa*), an opportunistic pathogen, contributes to high mortality rates in CF. The prevalence of *P. aeruginosa* lung infection gradually increases over time in CF patients from age 2 to 45 and *P. aeruginosa* eventually becomes the dominant strain. Therefore, we hypothesize that lower pH lung microenvironment contributes to the higher prevalence of *P. aeruginosa* infections. Our results indicated that an acidic environment significantly promoted bacterial biofilm formation and increased antibiotic resistance of *P. aeruginosa* . The increased bacterial virulence was confirmed by increased expression of biofilm/drug-resistance related genes in *P. aeruginosa* . We further determined *P. aeruginosa* infection could be ameliorated by increasing pH in the CF lung microenvironment. Ouabain, an ATP12A inhibitor, was able to increase pH in cultured CF epithelial cell from acidic to neutral, effectively decreased the bacterial number of *P. aeruginosa* . Our results indicated that pH in a microenvironment is an important factor for *P. aeruginosa* -associated lung infection in CF patients and treatments aim at increasing lung pH, such as Ouabain, are potential candidates to alleviate *P. aeruginosa* infections in CF patients.
85	Kimberly Lin	Translational Life Science	The Impact of Role Conflict on Pediatricians' Perceptions of Behavioral Health Care Services in Primary Care	Kimberly Lin, BS; David J. Kolko, PhD	While collaborative care models (CCMs) are well-established in the adult population, no standardized model yet exists in pediatric primary care. The organizational change introduced by CCMs poses a barrier to its more widespread use. We performed a study to better understand the effect of such a practice's existing organizational climate on pediatric primary care providers' (PCP) implementation of CCMs. 8 pediatric primary care practices (74 PCPs) in Pittsburgh, PA were randomized to 1 of 2 BH care practice interventions: Doctor-Office Collaborative Care (DOCC), which offers on-site integrated BH services delivered by a care manager (n=31 PCPs); or enhanced usual care (EUC), in which a care manager provides psychoeducation and makes a facilitated referral to a local behavioral health (BH) provider (n=43 PCPs). Surveys administered every 6 months assessed PCP perceptions of BH care practices and role conflict experienced in the practice. We find that pediatric PCPs who experience high role conflict in their practices have more positive perceptions of integrated BH services after delivering these services over time. These results suggest that PCPs in more stressful organizational settings may be more motivated to change their delivering of BH care services to a more effective and collaborative system.

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52	Chong Liu, PhD	Physical Science and Engineering	Ligand Exchange Phenomena and the Realization of Gradients within Metal-Organic Frameworks	Chong Liu, PhD; Tian-Yi Luo; Nathaniel L. Rosi, PhD	Many complex systems (e.g. cells, internal combustion engines, etc.) have compartmentalized structures. The performance of these systems relies on the different compartments working together, and the directional transport of matter (e.g. molecules, fuel, etc.) between compartments. We are motivated by such systems and aim to construct molecular materials capable of directional transport of matter. We are developing methods for constructing metal-organic frameworks (MOFs) that exhibit directional porosity and functionality gradients throughout their structures, with the ultimate goal of designing porous materials that can control the directional flow of molecules to specific locations for the purposes of sensing, catalysis, separations, etc. Here, we report our progress on developing pore-expansion based ligand exchange methods to prepare MOFs bearing porosity gradients. We studied the ligand exchange process and determined that shorter ligands are replaced by longer ligands in an outside□in fashion, where ligands on the crystal periphery are replaced first and the exchange process gradually migrates to the crystal core. By halting the ligand exchange reaction before completion, we isolated crystals bearing a porosity gradient. This MOF modification method promises gradual property shift inside porous crystals, which may lead to controllable transport and enrichment of guest species.
53	Chenxu Liu	Physical Science and Engineering	Measurement Induced Entanglement and 2-qubit Unitary Gates Using NV Centers in Diamond	Chenxu Liu, PhD; Gurudev Dutt, PhD; David Pekker, PhD	We proposed methods to achieve quantum entanglement of two local vibronic modes around Nitrogen-vacancy (NV) centers and entanglement of two spin-states of NV centers in separated diamond crystals. By detecting one Raman photon from two indistinguishable NV centers, we can achieve entanglement between local phonons around these two NV centers or the spin states of the NV centers. The fidelity of the entangled state can approach one in the week excitation limit. We also proposed a method to achieve two-qubit unitary gates heralded by a Raman photon using NV center electronic spin states, which pave the way for solid state quantum computing using NV centers.
54	Tianyi Luo	Physical Science and Engineering	Rational Design, Synthesis, and Covalent Postsynthetic Modification of pcu MOFs Based on Rare Earth M4(μ3-OH)4 Clusters	Tianyi Luo, Svetlana V. Eliseeva, Chong Liu, Patrick F. Muldoon, Stéphane Petoud, and Nathaniel L. Rosi	Taking advantage of the Td point group symmetry of distorted cubane rare earth metal clusters M4(μ3-OH)4, we designed and synthesized a series of isoreticular metal-organic frameworks featuring pcu topology with eight different rare earth metals (Y3+, Gd3+, Tb3+, Dy3+, Ho3+, Er3+, Tm3+, Yb3+) and the amino benzenedicarboxylate linker. Although they share the same topology as the prototypical IRMOFs that feature the Zn4(μ4-O) secondary building unit (SBU), this series has unique properties based on the rare earth SBUs. The X-ray crystal structure shows the potential of open co-ordination sites on the RE3+, and ion exchange experiments show that the frame-works are positively charged. Moreover, with these MOFs, we show that RE3+ sensiti-zation can be carefully adjusted via covalent postsynthetic modification.
55	Emily Marshman, PhD	Physical Science and Engineering	Developing a Quantum Interactive Learning Tutorial (QuILT) on a Quantum Eraser	Emily Marshman, Chandralekha Singh	We have developed a quantum interactive learning tutorial (QuILT) on a quantum eraser for students in upper-level quantum mechanics. The QuILT exposes students to contemporary topics in quantum mechanics and uses a guided approach to learning. It adapts existing visualization tools to help students build physical intuition about quantum phenomena and strives to help them develop the ability to apply quantum principles in physical situations. The quantum eraser apparatus in the gedanken (thought) experiments and simulations that students learn from in the QuILT uses a Mach-Zehnder Interferometer with single photons. We also discuss findings from in-class evaluations.

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6	Zehra Mehdi	Basic Life Science	Rad55 Phosphorylation Promotes Rad55 Interaction with csm2	Zehra Mehdi; Braulio Bonilla, MS; Kara A. Bernstein, PhD	Double-stranded DNA breaks are deadly for cells because they can lead to mutations that may eventually develop into cancer. Cells repair double-stranded DNA breaks. Homologous recombination (HR) is an error free pathway that can be used to repair double strand breaks. HR uses many proteins. Csm2 is a protein that is part of the Shu complex and interacts with Rad55. Rad55 and Csm2 can physically interact. Interestingly enough, Rad55 becomes phosphorylated upon treatment with the DNA-damage agent MMS. We hypothesize that Rad55 phosphorylation is the driving force to allow Csm2 to interact with Rad55. To test this hypothesis, we generated mutants of Rad55. Evaluation of the effect of these mutations on Rad55 and Csm2 were seen using protein-to-protein interaction by yeast two-hybrid systems. Our hypothesis was not fully supported because not all three serine sites were mutated. Therefore, once all three sites are mutated, we will be able to see if Rad55 phosphorylation drives the interaction with Rad55 and Csm2. The results gathered from this experiment will help further understand how Rad55 is recruited to DNA functions, how the Shu complex regulation takes place, and how HR is regulated.
56	David Meyers	Physical Science and Engineering	Current Enhancement by Injection into a Polariton Condensate	David Myers; Burcu Ozden; David Snoke; Loren Pfeiffer; Ken West	Condensation of exciton-polaritons has been extensively demonstrated in recent years. These polaritons are bosons that result from coupling trapped microcavity photons with quantum well excitons. This effectively results in photons that have been dressed with mass and repulsive interactions. We fabricated ≈ 100 μm × 100 μm square pillars to confine the polaritons, and then drove in-plane current through the polariton region by placing contacts on opposite sides of the pillars. The use of identical contacts on both sides resulted in an n-i-n structure, allowing injection of current of only one polarity. We report stimulated injection of free carriers into polariton condensates trapped in these pillars. We also show that this results in a back action on the current, leading to enhanced current flow when injected into a condensate.
57	Sunayana Mitra	Physical Science and Engineering	Understanding Ultrafast Proton Transfer Dynamics in Protic Ionic Liquids	Sunayana Mitra, Clinton Johnson, Kai Gronborg, Anthony W. Parker, Paul Donaldson, Sean Garrett-Roe	Protic ionic liquids (PILs) are molten salts of Brønsted acid and Brønsted base at room temperature. Promising characteristics of PILs like high thermal stability, low vapour pressure, high proton conductance and “water-like” hydrogen-bonding make them favorable candidates for next generation fuel cells. A question that still needs addressing is the mechanism of proton transport in PILs. Our hypothesis is that proton transfer in PILs undergo proton hopping called Grotthuss transport mechanism of transport. A photoacid, 8-hydroxypyrene-1,3,6-trisulfonic acid (HPTS), transfers a proton on a ps timescale when electronically excited with 400 nm light. With Time-Resolved Multiple-Probe Spectroscopy (TRMPS), the rise of the formic acid band in ethylammonium formate (EAF) indicates proton transfer from the photoacid in a PIL. The kinetic modelling of HPTS, HPTS*, PTS-*, PTS- and formic acid IR bands will elucidate proton transfer dynamics in PILs through a Grotthuss mechanism. A clear mechanistic picture of proton transport will help advancement in development and application of PILs for chemical synthesis and proton conducting electrolytes.

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59	Soumitra Mokashi Punekar	Physical Science and Engineering	Tunable Peptide Constructs for Systematically Controlling the Structure and Assembly of Chiral Gold Nanoparticle Single Helices	Soumitra Mokashi Punekar, Andrea D. Merg, Nathaniel L. Rosi	Chiral gold nanoparticle superstructures have attracted much interest because of their potential applications in novel optical devices and chiroptical sensors. Assembly methods are required to i) construct these materials and ii) carefully tune their structural parameters in order to optimize properties. Peptide-based methods for controlling the assembly of nanoparticles into chiral superstructures have been developed. These methods employ peptide conjugate molecules that consist of a gold-binding peptide (PEPAu=AYSSGAPPMPPF) attached to an organic tail (e.g. aliphatic chain or π-conjugated molecule); these constructs associate to the nanoparticles and direct their assembly. In this work, we prepare a series of divalent peptide conjugate molecules, Cx-(PEPAu)2 (x = 14-22). We examine peptide conjugate assembly behavior using FTIR and CD spectroscopy; we show how the peptide conjugates can direct the assembly of chiral single-helical gold nanoparticle superstructures. In particular, we study the effect that aliphatic tail length has on the assembly of the conjugates and ultimately the assembly and structural parameters (e.g. pitch, nanoparticle diameter and aspect ratio, etc.) of the gold nanoparticle single helices. Importantly, we show that fine adjustment of and control over peptide conjugate assembly allows for careful control over the structure of the chiral nanoparticle assemblies.
60	Jessica Montone	Physical Science and Engineering	Nanomechanical Probes of Sketched LaAlO3/SrTiO3 Single-Electron Transistors	Jessica Montone; Feng Bi, PhD; Mengchen Huang, PhD; Jung-Woo Lee, PhD; Hyungwoo Lee, PhD; Chang-Beom Eom, PhD; Patrick Irvin, PhD; Jeremy Levy, PhD	Nanoscale devices that manipulate single electrons present an exciting platform for the observation of electronic and mechanical effects. By utilizing the locally tunable metal-insulator transition at the interface of LaAlO3/SrTiO3, we can create single-electron transistors using conducting atomic force microscope (c-AFM) lithography. The piezoelectric nature of LaAlO3/SrTiO3 gives way to an expected coupling between mechanical motion and electric charge within the device. We can test this effect by applying pressure to the device using an insulating AFM tip while measuring changes in electron density. A cryogenic AFM system is used to examine these effects, as many of the most interesting properties of these devices are only observed at low temperatures.
7	Amitava Mukherjee, PhD	Basic Life Science	Asparagine Synthetase is Highly Expressed in the Pancreas and Pancreatic Acinar Cell ASNS is Upregulated with Asparaginase Exposure to Mitigate Cellular Injury	Amitava Mukherjee, PhD; Nayyar Ahmed, PhD; Fateema Turay, MD; Tanveer A Javed, BS; Li Wen, MD, PhD; Sohail Z. Husain, MD	The leukemia drug asparaginase causes pancreatitis in 6-10% of users, and this iatrogenic complication is a major issue for event-free survival. Thus, there is a crucial need to decipher the mechanisms underlying asparaginase-associated pancreatitis (AAP). Asparaginase functions primarily to deplete asparagine. We hypothesized that most asparaginase users (90-94%) do not develop pancreatitis because they can upregulate the counter regulatory enzyme asparagine synthetase (ASNS) and replenishes asparagine. Here we characterized the importance of ASNS in maintaining pancreatic homeostasis. In mice and humans, we demonstrate, ASNS is predominantly expressed in the pancreas. Asparaginase exposure in mouse (266-6) and rat (AR42J) pancreatic acinar cell lines caused a time- and concentration- dependent increase in ASNS expression. ASNS was also upregulated in primary mouse and human acinar cells with asparaginase. ASNS induction was unique to asparaginase, since other pancreatitis stimuli failed to induce ASNS. Further, ASNS knockdown caused pancreatic acinar cell injury and compounded by asparaginase, while ASNS overexpression protected 266-6 cells at baseline and from asparaginase induced injury. Taken together, pancreatic ASNS maintains acinar cell homeostasis at baseline and its upregulation is required to mitigate asparaginase-induced pancreatic cell injury. Therapies that augment pancreatic ASNS could be used to rescue the problem of AAP.

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61	Patrick Muldoon	Physical Science and Engineering	Confinement of Π-Systems in LNIII-Based Metal-Organic Frameworks Tunable Molecular Antennae for Photosensitization of Luminescent Materials	Patrick Muldoon; Svetlana Eliseeva, PhD; Tian-yi Luo; Stephane Petoud, PhD; Nathaniel Rosi, PhD	Lanthanide luminescence can be applied to numerous applications, and each application can require different photosensitization wavelengths. Our goal is to design and construct platform lanthanide MOF materials that can be systematically tailored for various applications. An approach that uses simple molecules to build complex tunable antennae within MOFs would provide a general means for sensitizing lanthanides in MOFs over a range of possible excitation wavelengths. We aim to develop a MOF-supported “ship-in-a-bottle” synthetic approach to assemble discrete molecular building blocks into extended π-systems confined within a MOF. Herein, functionalized oligoacetylene is grown within the pores of Ytterbium-based MOFs. These π-conjugated systems are covalently bound to the organic linkers of the MOF, and the resulting material exhibits visible light absorption (up to 700 nm) which sensitizes the near-IR emission of ytterbium in the MOF. The absorption spectra of these organic species are shown to be confinement-dependent.
62	Aditi Nethwewala	Physical Science and Engineering	Hall Conductance of 1D Electron Waveguides at the LaAlO3/SrTiO3 Interface	Aditi Nethwewala; Anthony Tyler Tyler, PhD; Yuhe Tang; Jianan Arthur Li; Hyungwoo Lee; Jung-Woo Lee; Chang-Beom Eom, PhD; Patrick Irvin, PhD; Jeremy Levy, PhD	We investigate Hall resistance in 1D electron waveguides. The well-known phenomenon of quantized Hall resistance in 2D electron gases is believed to be due to edge modes. We create electron waveguides at the LaAlO3/SrTiO3 (LAO/STO) interface using conductive atomic force microscopy lithography. An electron waveguide consists of a 1D channel with two weak barriers that allow us to change the chemical potential of the waveguide. We have observed ballistic transport in such devices by measuring the four-terminal longitudinal resistance. By creating transverse voltage probing leads inside the gated region of the waveguide, in order to measure its Hall resistance, we will explore the interplay between confinement potential and magnetic field, potentially allowing us to transition between 1D waveguide modes and 2D edge states in this class of devices.
63	Humair Omer	Physical Science and Engineering	Computational Study of Ni-catalyzed C-H Functionalization Reactions	Humair M. Omer; Kay Brummond, PhD; Peng Liu, PhD	The mechanisms of Ni-catalyzed C−H arylation, alkylation, and sulfenylation with N,N-bidentate directing groups are inves-tigated using density functional theory (DFT) calculations. While the C−H cleavage occurs via the concerted metalation-deprotonation (CMD) mechanism in all types of reactions, the subsequent C−C and C−X bond formation steps may occur via either oxidative addition to form a Ni(IV) intermediate or radical pathways involving Ni(III) complexes generated from homolytic dissociation of disulfides/peroxides or halide-atom transfer from alkyl halides. DFT calculations revealed that radical mechanisms are preferred in reactions with sterically-hindered coupling partners with relatively low bond dissociation energies (BDE) such as dicumyl peroxide, heptafluoroisopropyl iodide and diphenyl disulfide. In contrast, these radical pro-cesses are highly disfavored when generating unstable phenyl and primary alkyl radicals. In such cases, the reaction pro-ceeds via an oxidative addition/reductive elimination mechanism involving a Ni(IV) intermediate. These theoretical insights into the substrate-controlled mechanisms in the C−H functionalizations were employed to investigate a number of experi-mental phenomena including substituent effects on reactivity, chemo- and regioselectivity and the effects of oxidant in the intermolecular oxidative C−H/C−H coupling reactions.
64	Yun-Yi Pai	Physical Science and Engineering	One-Dimensional Nature of Pairing and Superconductivity at the LaAlO$_3$/SrTiO$_3$ Interface	Yun-Yi Pai, Hyungwoo Lee, Jung-Woo Lee, Anil Annadi, Guanglei Cheng, Shicheng Lu, Michelle Tomczyk, Mengchen Huang, Chang-Beom Eom, Patrick Irvin, Jeremy Levy	We examine superconductivity in LaAlO3/SrTiO3 channels in which the channel width transitions from the 1D to 2D regime. The superconducting critical current is independent of the channel width and increases approximately linearly with the number of parallel channels. Signatures of electron pairing outside of the superconducting phase are also independent of channel width. Collectively, these results indicate that electron pairing and superconductivity exist at the boundary of these channels and are absent within the interior region of the channels. The intrinsic 1D nature of superconductivity at the LaAlO3/SrTiO3 interface imposes strong physical constraints on possible electron pairing mechanisms.

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8	Sree Pulugulla, MS	Basic Life Science	Transcription of the IL1B Gene in Human CD3/CD28-Activated CD4 T Cells is Distinct from that of LPS-Treated Monocytes	Sree H Pulugulla; Thomas A Packard, PhD; Nicole l.K. Galloway, PhD; Gilad Doitsh, PhD; Juraj Adamik, PhD; Deborah L Galson, PhD; Warner C Greene, PhD; and Philip E Auron, PhD;	Interleukin 1β is a pro-inflammatory cytokine important for both normal immune responses and numerous chronic inflammatory diseases. Transcription of IL-1β activity has been extensively studied in stimulated myeloid cells, but not in lymphoid-derived CD4 T cells, the primary cellular target for infection by HIV. The rapid and vigorous increase in IL1B gene transcription for stimulated monocytes has previously been associated with the presence of pre-bound promoter Spi-1/PU.1, a myeloid-lineage transcription factor. We observed a significant increase in both IL1B transcription and translation in ex vivo CD3/CD28-activated and in vivo-differentiated CCR5+ memory CD4 T lymphocytes, despite the lack of detectable Spi-1/PU.1 at the IL1B promoter. This increase correlates with stimulatory epigenetic changes in CD4 T cells. Unlike stimulated monocytes, CD3/CD28-activated CD4 T cells possess bivalent H3K4me3+/H3K27me3+ nucleosome marks at the IL1B promoter, reflecting low transcriptional activity. This observation contrasts with the rapidly activated and extremely robust H3K4me3 monovalent IL1B gene promoter in TLR4-activated monocytes. We propose that in CD4 T cells, IL1B is transcribed from a low-activity bivalent promoter independent of Spi-1/PU.1. Accumulated cytoplasmic proIL-1β may ultimately be cleaved to mature 17 kDa bioactive IL-1β, regulating T cell polarization and pathogenic chronic inflammation.
65	Jonathan Ruffley	Physical Science and Engineering	Hybrid Stratified MOF-Plasmonic Nanoparticle Materials for Detection and Destruction of Chemical Agents	Jonathan Ruffley; Karl Johnson, PhD	There is a pressing need for materials capable of rapidly detecting and destroying chemical warfare agents. Stratified metal-organic frameworks (MOFs) containing plasmonic nanoparticles may be able to meet this need. Stratified MOFs consist of layered materials having different functional groups in each layer, which provide a gradient of functional groups to direct transport of target analytes to the MOF core. We seek to develop a detailed understanding of the fundamental properties of sorption, transport, photodetection, and photocatalytic degradation of target chemical species in stratified hybrid MOF-nanoparticle systems.
66	Huiling Shao	Physical Science and Engineering	Computational Study of Photo- and Redox-switchable Ring Opening Metathesis Polymerization and Ring Closing Metathesis	Huiling Shao; Aaron J. Teator, PhD; Dominika N. Lastovickova, PhD; Gang, Lu, PhD; Christopher W. Bielawski, PhD; Peng Liu, PhD	In collaboration with Christopher Bielawski research group, we conducted a series of calculations study the reaction mechanism of ROMP of cyclooctdiene and norbornene with the second generation Hoveyda-Grubbs catalysts bearing photo- and redox-switchable N-heterocyclic carbene ligands. These catalysts are capable of undergoing reversible transformation between two different states in response to external stimuli such as light and redox reagents. In other words, one will be able to control the state of the catalyst by changing light condition or adding redox reagent to the reaction mixture, which will later lead to a change in reaction outcome. Our group performed density functional theory calculations to investigate the reaction mechanisms as well as the effects of switchable ligands on reactivity. First, we compute the energy required for each elementary step in the reaction and construct the energy profile to locate the rate-determining transition state. We then evaluate the electronic and steric property of the switchable ligand to identify the salient factor that lead to the observed reactivity difference. The computational results suggested the reactivity of the switchable catalysts depends on the electronic and steric properties of the ligand and also the nature of the rate-determining step.

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86	Eric Strobl, PhD	New Research Tools and Techniques	Causal Discovery under Non-Stationary Feedback	Eric V. Strobl, Shyam Visweswaran	Causal discovery algorithms help investigators infer causal relations between random variables using observational data. In this project, we relax the acyclicity and stationary distribution assumptions imposed by the Fast Causal Inference (FCI) algorithm. We provide two major contributions in doing so. First, we introduce a representation of causal processes called Continuous time Markov processes with Jump points (CMJs) which can model continuous time, feedback loops, and non-stationary distributions. Second, we characterize constraint-based causal discovery under the CMJ framework using mixture data, or data created by sampling from a variety of unknown time points from the CMJ. The CMJ may for example correspond to a disease process, and the samples in a mixture dataset to cross-sectional data of patients at different stages in the disease. We finally propose a sound modification of FCI called the Fast Causal Inference with Feedback (F2CI) algorithm which uses conditional independence testing and conditional mixture modeling to infer causal structure from mixture data even when feedback loops, non-stationary distributions, selection bias and/or latent variables are present. Experiments suggest that the F2CI algorithm outperforms FCI by a large margin in correctly identifying causal relations when non-stationary distributions and/or feedback loops exist.
67	Erin Sutton	Physical Science and Engineering	Sum and Difference Frequency Generation in a LaAlO3/SrTiO3 THz Nanodetector	Erin Sutton, Lu Chen, Patrick Irvin, Jeremy Levy	We investigate the broadband nonlinear detection capabilities of nano-junctions created at the interface of LaAlO3/SrTiO3 heterostructures. Using conductive AFM lithography, we define a nano-junction at the interface. We then illuminate the junction with an ultrafast femtosecond pulse laser. Due to the nanometer-scale size of the junction and the femtosecond duration of the ultrafast pulse, optical fields are localized in time and in the plane of the junction. As a result of the large third-order nonlinear susceptibility at the nano-junction, the polarization of the resulting THz field combines the spatial resolution of a bias voltage and the temporal resolution of the optical field. Using a pulse shaping setup with a dual-mask spatial light modulator, we shape the incoming pulse so that two wavelengths are maximized, and the rest suppressed. The nonlinear THz generation at the nano-junction enables broadband sum and difference frequency generation of these two wavelengths that is limited in range and resolution only by the spectral width of the femtosecond pulse.
68	Yuhe Tang	Physical Science and Engineering	Non-Coulombic Frictional Drag Currents in Coupled LaAlO3/SrTiO3 Nanowires	Yuhe Tang, MS; Anthony Tylan-Tyler, PhD; Hyungwoo Lee, PhD; Jung-Woo Lee, PhD; Michelle Tomczyk, PhD; Mengchen Huang, PhD; Chang-Beom Eom, PhD; Patrick Irvin, PhD; Jeremy Levy, PhD	Frictional drag phenomena are investigated in coupled nanowires formed at LaAlO3/SrTiO3 heterointerfaces. The weak decay of drag resistance with increasing wire separation rules out Coulomb interactions as the coupling mechanism. The observed unidirectional current drag is explained using a simple model that invokes slight asymmetries within the nanowires. These results provide new insights into non-Coulombic electron-electron interaction effects that must be accounted for in any full description of electron transport at oxide interfaces.

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9	Maiwase Tembo	Basic Life Science	PIP2 and Ca2+ are Both Required to Open TMEM16a Channels in *Xenopus laevis* Oocytes	Maiwase Tembo and Anne E. Carlson	The widely expressed Ca2+- activated Cl- channel, transmembrane member 16A (TMEM16a), has various physiological functions ranging from mucosal secretion to regulating smooth muscle contraction. Despite its importance, little is known about the mechanisms that regulate TMEM16a gating. Here we recorded Ca2+-evoked Cl- currents passed by the endogenous TMEM16a in oocytes from the African clawed frog, *Xenopus laevis* . Using the inside-out patch clamp technique, we observed that the TMEM16a-conducting currents rundown despite the continued presence of Ca2+. Current rundown is common amongst channels regulated by phosphatidylinositol 4,5-bisphosphate (PIP2). Thus, we tested the hypothesis that TMEM16a is potentiated by PIP2 using PIP2 sequestering and recovering agents. First, we recorded repeatable current rundown seconds after patch excision in the presence of Ca2+. After current had run down, we applied the soluble dioctanoyl-PIP2 analog (diC8-PIP2) in the presence of Ca2+ and we observed 40 % current recovery. Conversely, neither diC8-PIP2 with no Ca2+, nor diC8-PI without the two phosphate groups, were able to recover current. We next applied PIP2 sequestering agents, neomycin and anti-PIP2, and found that TMEM16a current ran down twice as fast than when exposed to just Ca2+. Altogether, our data demonstrate that TMEM16a requires both Ca2+ and PIP2 to pass current.
10	Yaqun Teng	Basic Life Science	CSB Cooperates with RAD52 in Transcription-Coupled Recombinational Repair	Yaqun Teng; Satoshi Nakajima, PhD; Zhuobin Liang, PhD; Patrick Sung, PhD; Arthur S. Levine, MD; Li Lan, MD, PhD	Transcribed genomic loci are prone to breakage and instability. Transcription-coupled homologous recombination (TC-HR) is a recently discovered novel mechanism by which DNA double-strand breaks (DSB) at transcriptionally active loci are preferentially repaired via an error-free recombinational repair. We recently identified that Cockayne Syndrome protein B (CSB) is required for the efficient damage response of recombinational repair factor RAD52, while the mechanism of how CSB coordinates with RAD52 in TC-HR is still unknown. To pursue the mechanism, we created CSB CRISPR-Cas9 knock out (KO) cells. CSB KO leads to decreased RAD52 damage response and increased sensitivity to ionizing radiation (IR). We further identified that CSB interacts with RAD52 via its acidic domain (337-509 a.a.), and interacts with RNA POLII via its 961-1399 a.a. region. Both domains are recruited to transcriptionally active damage site. More importantly, the acidic domain could partially rescue the cell survival after IR and RAD52 recruitment in CSB KO cells. Mutation of the acidic amino acids within the acidic domain stabilizes its interaction with RAD52 both in vivo and in vitro, suggesting that structural features but not the acidic amino acids in acidic domain might be critical for the RAD52 interaction and its function in TC-HR.
69	Binbin Tian	Physical Science and Engineering	Phases and Transport in Spin- and Mass-imbalanced Fermi Mixtures in One Dimension	Binbin Tian, Yuchi He, Michelle Tomczyk, Megan Kirkendall, Anthony Tylan-Tyler, Patrick Irvin, Jeremy Levy, Roger Mong, David Pekker	We studied numerically the rich phases of spin- and mass-imbalanced Fermi mixtures in one dimension. Together with experimental group, we simulated transport properties for LAO/STO systems.
70	Minh Nguyen Vo	Physical Science and Engineering	Quantum Chemical Insights into the Mechanism of AlCl3/H2O Catalyzed Polymerization of Isobutylene	Minh Nguyen Vo; Yasemin Basdogan; Bridget S. Derksen; John A. Keith, PhD; Nico Proust; G. Adam Cox; Cliff Kowall; J. Karl Johnson, PhD	We performed molecular level studies on the initiation and propagation mechanisms of isobutylene polymerization (IB) with AlCl3/H2O based catalyst. Using the growing string method, we identified AlCl3HOHAlCl3 as a potential initiator com-plex with low reaction barrier for both initiation and propagation pathways, which are consistent with experimental conditions. Contrary to the putative textbook mechanism, we demonstrated that a complex of one AlCl3 and one H2O molecule cannot initiate the reaction due to high-energy barrier associated with transferring the proton directly from the H2O to the IB group. At least two AlCl3 and one H2O molecule is necessary to initiate the reaction.

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18	Janet Wang	New Research Tools and Techniques	Specifically Differentially Expressed Genes between Breast Invasive Lobular Carcinoma and Invasive Ductal Carcinoma Suggest Distinct Biology	Janet Z. Wang; David N. Boone, PhD; Andrew Warburton	Despite its high prevalence and relatively poorer prognosis, invasive lobular carcinoma (ILC) remains understudied compared to the more common histological subtype of breast cancer, invasive ductal carcinoma (IDC). Others have described mutation and signaling differences between ILC and IDC, but we hypothesize that the identification of differentially expressed genes (DEGs) between the two subtypes will provide additional insight into the biology of ILC and potentially lead to the development of biomarkers for its early detection. We used publicly available reanalyzed TCGA counts data due to its inclusion of long noncoding RNAs (lncRNAs), functionally important biomarkers in breast cancer. We identified DEGs by performing DESeq2 analyses of ILC estrogen receptor positive (ER+) tumors (191 samples) vs. normal (113 samples), IDC ER+ tumors (562 samples) vs. normal (113 samples), and ILC ER+ tumors vs. IDC ER+ tumors and filtering (FDR < 0.001, fold change >= 1.5, TPM > 1). The results of the hierarchical clustering showed that the ILC-specific and IDC-specific differentially expressed protein-coding and lncRNA genes grouped patients into ILC, IDC, and normal subtypes better than protein-coding genes alone. Ingenuity Pathway Analysis demonstrated that ILC-specific genes are involved in immune response and signaling pathways and are regulated by vitamin D3.
11	Katherine Wozniak	Basic Life Science	The Depolarizing Current of the Fast Block to Polyspermy in *Xenopus laevis* is Mediated through TMEM16a	Katherine L. Wozniak and Anne E. Carlson	Preventing polyspermy, the fertilization of an egg by multiple sperm, is essential for the normal embryonic development of most animals. In external fertilizers, a depolarization of the egg membrane serves as the most immediate barrier to inhibit sperm from entering an already fertilized egg, a phenomena known as the fast block to polyspermy. In the African clawed frog *Xenopus laevis* , the fast block requires an increase of cytosolic Ca2+ and an efflux of Cl- to depolarize the egg. We tested the hypothesis that the fast block in *X. laevis* activates the Ca2+-activated Cl- channel TMEM16a. TMEM16a is abundant in immature *X. laevis* oocytes; however, we do not know whether the channel is present in fertilization-competent eggs. We screened various small molecular inhibitors of TMEM16a for their efficacy at blocking *X. laevis* TMEM16a (xTMEM16a). We then utilized the two most potent xTMEM16a inhibitors, MONNA and Ani9, to assess the requirement of TMEM16a for the fast block by performing whole cell recordings during fertilization. We found that xTMEM16a inhibitors slowed or completely inhibited the fertilization-evoked depolarization. These results suggest that TMEM16a is present in *X. laevis* eggs and is activated by fertilization to evoke the fast block to polyspermy.
75	Hao Wu	Physical Science and Engineering	Kitaev Model with Quantum Dot Chains in InSb Nanowires	Hao Wu; Zhaoen Su; Jun Chen; Peng Yu; David Pekker; Moira Hocevar; Diana Car; Sebastien Plissard; Erik Bakkers; Sergey Frolov	We experimentally explore whether chains of quantum dots in semiconductor nanowires can be used to emulate important one-dimensional Hamiltonians such as the topological p-wave superconductor. We examine the building block of the Kitaev model by establishing a double quantum dot with superconducting contacts in an InSb nanowire. We demonstrated that Andreev-bound states in each dot hybridize to form the double-dot Andreev molecular states. We showed the parity and the spin structure of Andreev molecular levels. Understanding Andreev molecules is a key step towards building longer chains which are predicted to generate Majorana-bound states at the end sites. Next, we have implemented a triple quantum dot chain in an InSb nanowire where each dot is tuned to be strongly coupled to a separate NbTiN superconducting lead. We have studied transport through Andreev-bound states on individual dots, dot pairs and entire triple dot. We explore the influence of Coulomb energy on the Andreev spectra of the chain. We use magnetic fields parallel to the nanowire axis to study field dependence of the triple dot Andreev-bound states. We observe zero bias conductance peaks that appear at finite applied magnetic fields, and as split peaks.
76	Xinyi Wu	Physical Science and Engineering	Breaking Electron Pairs in Pseudogap State in STO/SmTO/STO Quantum Wells	Xinyi Wu; Arthur Li; Megan Kirkendall; Patrick B. Marshall; Susanne Stemmer, PhD; Patrick Irvin, PhD; Jeremy Levy, PhD	Pseudo-gaps have been found in strongly correlated, two-dimensional electron liquids in SmTiO3/SrTiO3/SmTiO3 quantum well structures at low temperature. We examine the existence of pre-formed electron pairs in the material by experimentally break them, creating mobile quasi-particles which will increase conductance in channels. Methods achieve this includes applying voltage bias larger than gap width, as large as 120mV in some of our samples, and optically exciting with infrared light. This will give more insight into possible electron pairing mechanism and non-Fermi liquid behavior.

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77	Dengyu Yang	Physical Science and Engineering	Surface Acoustic Wave Generation and Detection on LAO/STO	Dengyu Yang, Yun-Yi Pai, Yang Hu, Hyungwoo Lee, Jung-Woo Lee, Chang-Beom Eom, Patrick Irvin, Jeremy Levy	The use of Surface Acoustic Waves (SAW) is potentially an effective method for single-electron transport, which is an emerging option for quantum information transfer. We aim to observe SAW in LAO/STO heterostructures. Using a positively/negatively-biased AFM tip, one can switch between the conducting and insulating phases of the material, thus creating or erasing nanowires in the structure. Using this method, interdigited transducers (IDT) can be created in the structure, which can convert electronic signals into acoustic signals and vice versa. Two IDTs are thus written on the structure as a generator and a detector. Due to material and dimensional constraint, a radio frequency electronic signal is used to maximize the effect. SAW can generate potential minima relying on the piezoelectric property of LAO/STO, and by changing position of these potential minima electrons can be transported along the nanowire.
78	Xiaoou Zhang	Physical Science and Engineering	Optical Selection Rule of Excitons in Gapped Chiral Fermion Systems	Xiaoou Zhang; Wenyu Shan, PhD; Di Xiao, PhD	We provide a systematic discussion on the optical selection rule for excitons in two dimensional gapped chiral fermion systems. We find that the angular momenta of bright and dark excitons are related to the winding number of the chiral fermion model and the crystal symmetry. Based on our theory, we propose that the s exciton states in magnetically doped surface state of a topological crystalline insulator and gated 3R-stacked MoS2 bilayers are optically dark. In the latter case, we further show that a gate voltage can be used to tune the s exciton state between dark and bright. This proposal provides a pathway to electrical control of optical transitions in two-dimensional material.