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PRESENTATION ABSTRACTS

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Ilya Belopolski: Physics, CC'12

Open questions in multi-messenger gravitational wave astronomy

Gravitational wave astronomy promises to forever alter our view of the universe by enabling us to observe astrophysical phenomena that are not directly associated with the emission of light. However, although the existence of gravitational waves was first predicted nearly one hundred years ago, they have not yet been directly detected. The Laser Interferometer Gravitational Wave Observatory (LIGO) is a network of phenomenally high-precision optical interferometers that detects minute distortions of space-time due to incident gravitational radiation of cosmic origin. By 2014, the second generation of LIGO interferometers, Advanced LIGO, will be operational and will incorporate upgrades that allow it to detect displacements of its long-arm optics as small as 10^{-21} meters, several orders of magnitude smaller than the diameter of a proton. The effective sensitivity of Advanced LIGO will be further improved by comparing gravitational wave data with astronomical observations from conventional light telescopes through so-called multi-messenger searches. Since many transient gravitational wave emissions coincide closely with E&M bursts, direct observation of the associated E&M signal can provide precise knowledge of the event time, the source location, and the source distance. This information allows gravitational wave searches to be more robust to detector glitches, reduces the computational power required for analysis, and yields more interesting physics by allowing estimates of the gravitational wave energy emitted at the source. As higher sensitivities are achieved through Advanced LIGO and as conventional light telescopes become ever-more precise, this multi-messenger approach offers us powerful observational tools to investigate fundamental problems in cosmology and astrophysics.

Here we survey the open questions in multi-messenger gravitational wave astronomy and evaluate the state of current research for several of the most provocative fields of investigation, as follows : (1) Are there regimes in which Einstein's theory of general relativity is violated? We consider, in particular, strong-field regimes such as those which characterize the imploding core of supernovae, the structure of rapidly-rotating neutron stars, and the final stages of the merger of two compact bodies. We also consider cosmological length scales, where a failure of general relativity might allow for the existence of the dark energy which appears to dominate the universe and drive its expansion. (2) Is the speed of propagation of gravitational waves less than, equal to, or greater than the speed of light? If gravitational waves propagate more slowly than light, could they be associated with a massive graviton and could these gravitons account for dark matter in the universe? Lastly, (3) do quark stars exist? How easily will Advanced LIGO be able to set upper limits on the quadrupole deformations of the pulsars which currently serve as possible quark star candidates? When will non-detection confront theoretical models of exotic matter? By evaluating current research on these fundamental problems, we hope to define directions for future work in the field.

Rohan Bhandari: Physics, CC'13

Observation of the Interlayer State in Graphene on Ir(111)

By analyzing and understanding the image states of graphene, one can gain insight into its electronic properties. An image state refers to an electron that has been excited outside of the surface of the metal, and its resulting electric field. Graphene is of particular interest, because it exhibits very curious electronic properties: its electrons are able to travel relatively far distances before colliding with other electrons. Also, these electrons behave as Dirac particles, essentially acting as particles in an accelerator, while

actually traveling relatively slowly and residing in a metal. From a better understanding of these properties, it is hoped that Graphene can be applied towards nanoelectronics and superconductors, among other fields.

The image states were probed through 2 Photon Photoemission of graphene that was grown on Iridium (111) by chemical deposition. This procedure uses a high frequency (on the order of a femtosecond) laser to bombard the graphene surface with photons, which can doubly excite the electrons. The resulting electron energies are measured and the original electron energy can then be inferred.

The collected data was then analyzed and fit with a Voigt curve, which is a convolution between a Gaussian and Lorentzian curve. By fitting the Fermi cutoff with a Fermi function, it was found that the experimental resolution was 40 meV. This resolution corresponds to the width of the Gaussian curve in the convolution, which is fixed. The analysis showed the existence of an interlayer state between the graphene and Iridium, which had been previously obscured due to resonance from the other image states.

Nathan Booth: Physics, CC'14
Electron transport in bilayer graphene

Graphene, which has attracted great interest in the scientific community and in the media in the past several years, is a two-dimensional substance consisting of a single atomic layer of carbon. Recent research has suggested that few-layer graphene also has properties worthy of exploration. The research discussed here explores electron transport in such substances—specifically, bilayer graphene. The samples used in these experiments were developed by exfoliating high-quality graphite pieces and pressing them down onto silicon chips. From there, areas of bilayer graphene were located on the chip and patterns for Hall bars were etched using electron beam lithography, and contacts were formed to match the pattern by evaporating gold onto the sample. Finally, the graphene was suspended in an electrolyte. We then did Hall measurements across the sample to measure its conductivity as temperature changed. We experimented with mixing lithium and other metals into the electrolyte and then cooling the system down to low temperatures to gauge how the Kondo effect changes the conductivity of the substance as the metal intercalates between the layers. This course of research may eventually lead to observation of superconductivity in graphene. So far the results have been promising and high conductivities have been seen, especially with samples that have lithium intercalated, but the research is ongoing and conclusive results remain to be seen.

Alice Chang: Chemistry, CC'13
Single-Molecule Conductance through Direct Au-C Contacts

The phenomenon of single-molecule conductance has potential applications to building molecular-scale electronics. In a few generations, the composition of electronic devices is expected to be controlled on the atomic scale; the ultimate miniaturization would use components that are single molecules. Molecular conductance junctions are nanoscale structures in which single molecules conduct electrical current between two electrodes. In such junctions, the contacts between the molecule and the electrodes determine current-voltage characteristics. One class of molecular conductors consists of compounds synthesized by attaching two linker groups to a conjugated molecular core. Strained rings in the linker

group can directly bind to the two gold electrodes used to measure conductance, allowing efficient charge transport across the molecular junction. Conductance through the linkers and core can be optimized by directing charge transport through a delocalized π -electron system, since conductance through σ -bonds alone is typically weak. The goal of this project is to explore π -conductance phenomena through simple strained single-molecule conductors that form direct Au-C contacts. Toward this goal, encouraged by DFT-predicted structures, we synthesized 1,4-dicyclobutenebenzene and 1,4-dicyclopentenebenzene in high purity (>99%) and submitted samples for STM-based break-junction conductance measurements. For both compounds, conductance measurements were on the order of $10^{-5} \times G_0$, where G_0 is the quantum of conductance through two gold electrodes in direct contact. Although the conductance is low compared to the conductances reported in the literature for molecules with known heteroatom linker groups (the conductance measured for 1,4-diaminobenzene, for example, is on the order of $10^{-2} \times G_0$), it is higher than expected considering that the electrodes form direct Au-C contacts with the strained-ring linkers. Such linkers have advantages over known linkers, such as improved stability and low toxicity, that would be crucial to applying single-molecule conductors to nanoscale electronics.

In order to further investigate properties of direct Au-C contacts, we plan to synthesize other strained molecules with novel linkers. Another extension of this project will be to measure the conductance of a family of straight-chain alkanes with the same strained linkers. The conductance G decays as $G \approx e^{\beta N}$, where β is the decay constant and N the number of methylene groups on the backbone; by measuring the conductances of linker-terminated alkanes with $N = 4, 6, 8$, or 10 methylene groups, we can compare the effectiveness of our novel strained-ring linkers to that of linkers discussed in the literature.

Vadim Chanyshv: Mathematics, CC'13
The St. Petersburg Paradox

The St. Petersburg Paradox is a relatively well known problem in game theory, which is famous for having no numerical solution. The problem describes a lottery game that is played by flipping a coin as many times as needed until it results in tails. Every time the coin is flipped, however, the payoff is doubled. The paradox of the problem is that the expected payoff is impossible to calculate. However, that does not mean that the game is not playable in practice. Working on this problem in the past I have found a way to estimate the expected payoff at certain confidence level, which is useful for finding the average loss the lottery can expect to have with each game it allows its customers to play.

This summer I have found a formula to calculate exactly what the chance is that the payoffs (the money it pays to its players after each round, for an unlimited number of rounds), which are a random variable, cross a diagonal boundary that represents the lottery's growing revenue. The complexity of this problem is that there is no way to calculate this exactly without making millions of calculations, which by hand would take an indefinite amount of time. The formula that I created in Excel, however, generates all the possible combinations of outcomes for any number of rounds and then calculates the probabilities of these outcomes occurring. With those values it is possible to calculate the probability that a boundary with any slope and intercept is crossed at any point. The formula itself is infinite in length and takes up an indefinite number of cells because no finite number of operations in an Excel spreadsheet can calculate an infinite number of probabilities that correspond to an infinite number of combinations. However, this is not an issue, because the formula not only generates new combinations for each round but also expands itself to

fit the required number of calculations for the task that it is given, which means that it is only limited by the speed of the processor in a computing machine.

Boundary crossing problems are well known, however, they have never been applied to the St. Petersburg Paradox in particular. The formula is extremely useful because it can easily be altered to make calculations for relevant sequences since there is nothing exceptional about the St. Petersburg Paradox other than an infinite expectation of outcomes. Finally the formula gives the exact risk a lottery experiences when letting the public play the game, which has never been calculated before. For example if a lottery has \$10,000, collects \$10 per game, it could use the formula to find out the probability that it will be bankrupt after 5000 games played. It can also find out other relevant information such as the probabilities that other boundaries (determined by the initial amount the lottery has and the price it collects) are crossed to know how its risk of going bankrupt will be affected by changing the price of the game or the initial amount of money it has in its savings. The formula I have developed, therefore, produces a business model for any lottery willing to install this or a game that has a similar structure.

Rena Chen: Astrophysics, CC'14

Optimized synthesis by chemical vapor deposition of atomic layer hexagonal boron nitride

Hexagonal boron nitride (*h*-BN) is a two dimensional material complementary to graphene that can be used to engineer devices with unusual electrical and optical properties such as high mobility electron transistors and far ultraviolet light emitting diodes. Recently, atomic layers of graphene with *h*-BN have been grown using chemical vapor deposition (CVD). CVD also produces high quality *h*-BN films that are thin, uniform, and continuous. Although *h*-BN films of two atomic layers have been demonstrated using CVD, we endeavor to produce monolayer *h*-BN. We used CVD to synthesize *h*-BN on copper and nickel substrate with ammonia borane as the precursor. The *h*-BN was characterized by Raman spectroscopy, atomic force microscopy, and transmission electron microscopy. Scalable synthesis of monolayer *h*-BN films using CVD, which can produce *h*-BN in large quantities at low costs, has the potential to galvanize further research in graphene electronics and the production of optoelectronic devices in industry.

Woo Chang Chung: Mathematics, Physics, CC'13

Characterization of the Charge Density Wave Phase in NbSe₂

Metals often undergo a phase transition to a new electronic state when they are cooled down to a low temperature; superconductivity is a well-known example of such transition. Another interesting example of an electronic phase transition occurring in low dimensional metals is the charge density wave (CDW). A CDW is a coupled periodic modulation of conduction electron density and atom positions in the lattice. For some low dimensional metals, the CDW state is more energetically favorable at low temperature than the metallic state. However, the true reason for the existence of the CDW state is not known for many materials. Most experimental measurements of the CDW we have thus far are from momentum space, which is the Fourier transform of real space. The goal of this experiment is to better understand how the CDW forms in the real space from the metallic state as the temperature of the material is lowered. The material of choice is two-dimensional metal NbSe₂, which is the most well studied CDW material so far, but one in which the reason for the CDW transition is still debated. Our scanning tunneling microscopy

(STM) data confirmed that CDW persists around crystal defects beyond the transition temperature (33.7 K). A part of the characterization of the CDW was to determine the relationship between the phase of the CDW near defects and the bias voltage applied to the sample crystal (= energy levels of the crystal). A set of tunneling spectroscopy maps with bias voltage ranging from -1.4V to 1.4V in intervals (or frames) of 0.05V was obtained. For each frame, CDW components were selected using 2D-FFT filtering. Then an autocorrelation analysis was performed between each frame and the CDW at bias = 1.4V, which was chosen as the reference. The autocorrelation analysis showed the variation of the CDW phase with applied bias giving us information on the effect of the CDW on the various energy bands of NbSe₂.

Kevin Guo: Mathematics, CC'15

Virus Classification with Hierarchical motif clustering

Molecular biologists will classify viruses based on its shape, form, and other phenotypical features. Relying solely on phenotype will capture large differences between viruses, but often will fail to capture any genetic nuances between the same family and strain. Using machine learning techniques, we seek to learn protein subsequences from a virus's genome that are strong classifiers of its host: plant, invertebrate, or vertebrate.

Our data consist of 146 virus sequences along with their designated hosts. This method uses a boosting algorithm modeled on an alternating decision tree (ADT). For each round of boosting, the algorithm searches for the weak rule that minimizes an exponential loss function on the dataset, which is strongly correlated with the accuracy of the classifier. After finding the weak rule, the algorithm attaches it to the ADT and continues to the next round of boosting. Each decision node of the ADT has two output nodes, with an associated $_$ and $\sim_$. When a virus's protein sequence is run through the ADT, if it passes the threshold of a decision node, $_$ is added to its score; otherwise, $\sim_$ is subtracted, with each virus's final score determining its classification based on our boosting model. More specifically, we first search for the top N protein subsequences (kmers) of length k whose exact matches classify the train set with the least exponential loss. We then convert each subsequence into a Position Specific Scoring Matrix (PSSM) smoothed by a machine epsilon. The PSSMs are clustered using Hierarchical Motif Clustering based on their "similarity", which is determined by a weighted, symmetric form of the Kullbacker-Leibler Divergence. The final step searches over $N-1$ PSSMs to find the PSSM, decision/output node, and threshold combination with the least exponential loss, compares it to the kmer with the least exponential loss, and choosing the lesser of the two to add to the ADT as the new weak rule.

Our method when tested with $k=8$ $N=10$ achieves a test accuracy of 92% when averaged across 5 rounds of cross validation. Unsurprisingly, the top 10 kmers were more than enough to seed the initial PSSMs. Greater values of N mostly decreased the test accuracy, although some upward spikes resulted. However, this was expected, since a greater number of seed kmers would lead to more variability. Previous techniques of classification involving machine learning did not use the probability distribution methods of the PSSM. Instead, it was necessary to specify a mismatch neighborhood m for each kmer with thresholds being a kmer match within m amino acids. The mismatch neighborhood attempts to capture the high rate of mutation in viruses, so that a mutation of one amino acid will not be discounted in the decision node. The mismatch method for $(k,m)=(8,0)$ yields very poor test accuracy (84%); however, when $m=1,2$ test accuracy improves dramatically to 95%. A confidence interval concerning the test accuracy reveals there is

no statistical difference in test accuracy between our Hierarchical Motif Clustering method and the previous mismatch neighborhood technique. It is necessary to generate a mismatch neighborhood array for each value of m ; when considering the number of candidate kmers, for large data sets, this step could take weeks. Hierarchical Motif Clustering only requires that we preprocess one array for $m=0$, while effectively capturing the mismatch neighborhood within its probability distribution. In addition, PSSMs often outperform individual kmers in terms of boosting loss even when the initial seed kmers are generated by $m=1$ or $m=2$. This indicates PSSMs are stronger at differentiating subtle differences in genetic data during later rounds of boosting than single kmers.

In further work, we will use different values of (k,m) to seed our Hierarchical Motif Clustering. The mismatch neighborhood method for larger values of k naturally requires larger values of m for decent accuracy. Although using $m=0$ to seed our model may no longer be accurate, we hope that Hierarchical Motif Clustering will significantly reduce the size of the mismatch neighborhood to be generated to get high test classification accuracy.

Jonathan Huggins: Computer Science, CC'12

The Structured Explicit Duration Infinite Hidden Markov Model

My research was in the area of statistical machine learning. I developed a novel statistical model, which I call the structured explicit duration infinite hidden Markov model (SED-iHMM). The SED-iHMM can be used to model data generated from a process evolving over time. For example, it could be used to model human speech or changes in the stock market. Usually, statical models have a fixed number of parameters that are adjusted to fit the data. My model is "non-parametric" (and is thus referred to as "infinite") because the number of parameters is automatically determined based on the data. Thus, if the data is simple, the SED-iHMM will have only a few parameters, whereas if the data is complex, the SED-iHMM will have many more parameters. In particular, for the SED-iHMM, there are an infinite number of "states" that the model transitions between. Because the model is trained on a finite amount of data, however, in practice the model only makes use of a finite number of states. The model only knows about its current state when it decides whether to transition to a new state, and, if so, which state to transition into. Each state has its own probability distribution of output values--these distributions are used to account for the observed data.

Many existing models can be described as special cases of the SED-iHMM. I focused my experimentation on a particular case of the SED-iHMM, which I call the explicit duration infinite hidden Markov model (ED-iHMM) and which had not previously been described. The ED-iHMM was able to successfully fit a range of datasets and produced equivalent, and in some cases superior, results to those of a related non-parametric model, the HDP-HMM. On a theoretical level, it places many other versions of the hidden Markov model in a more general conceptual framework. I expect that the SED-iHMM will be a useful tool because it is a flexible framework that allows for countless specializations capable of meeting practitioners' modeling needs.

Raina Jain: Biology, CC'15

The Effect of Bioglass Particle Size on Cell Response

With increasing life expectancy, a greater percentage of the population suffers from diseases that cause bone destruction. To replace defective bone, titanium implants are most commonly used, but they cause scarring and have a limited lifetime of about 15 years. In contrast, Bioglass ($45\text{SiO}_2\text{-}24.5\text{CaO-}24.5\text{Na}_2\text{O-}6\text{P}_2\text{O}_5$) appears more promising with superior biocompatibility. Currently, the majority of Bioglass implants are used in dental applications in the form of powder. Past research has shown an influence of particle size in the growth of bone in vivo, but no study has been conducted to understand and explain these findings with in vitro experiments. The goal of this study was to examine the effect of Bioglass particle size on cell behavior, both morphologically and quantitatively.

To examine the effect of Bioglass particle size on cell behavior, at first trials were conducted to establish an appropriate experimental procedure. Various types of adhesive substances (silicone, agarose, nail polish, cyanoacrylate, and epoxy) were tested for cell toxicity. Results from the trial experiments showed that silicone was the best material to use as an adhesive between the Bioglass particles and coverslip substrate, since it was neither toxic to cells nor bioactive.

The Bioglass powder was commercially produced with particle size ranging from 90 to 710 μm . The mixture of particles was further sieved into four size categories for a more precise assessment. Using silicone, Bioglass particles of various sizes were scattered on cover slips for biological experimentation with MC3T3 precursor osteoblasts. After the samples were sterilized, these cells were seeded and grown on particles of various sizes for multiple time-points. At appropriate times, the samples were removed and fixed with formaldehyde. Then, all samples underwent immunofluorescence staining for their nuclei, actin cytoskeleton, and vinculin (focal adhesion protein).

By means of fluorescence microscopy, the samples were imaged and the morphology of the cells was recorded to compare cell proliferation qualitatively as well as quantitatively with respect to Bioglass particle size. The nuclei of cells on Bioglass particles were imaged at a low magnification and counted manually. Morphologically, the cell shape appeared healthy in the majority of samples at all time-points. Cells on the smallest particle size, however, appeared rounded in shape, indicating a lack of compatibility with the surrounding environment. This observation was further confirmed by the quantitative analysis of cell growth. On the smallest particle size, over 3 days, cell numbers quickly dropped down to zero. Other trends in cell growth were also evident, with two of the larger size particle size showing a clear enhancement of cell proliferation. It appears that the concentration of dissolution products in culture medium, which depends on the surface area (hence also the size) of particles, reached a threshold toxic value for the finest powder, leading to complete cell death after one day. The larger size powder, however, appeared to promote cell growth. Further experiments are needed to establish the optimum particle size as a function of the ratio of particle surface area to culture medium volume.

Joon Ho Kang: Biophysics, CC'12

**Proteolytic machine studied at single-molecule level with Total Internal Reflection
Microscope/electromagnetic tweezer**

All cells employ ATP-fueled protease to regulate protein activity. In the Clp XP protease, Clp X recognizes particular protein sequences, unfolds and then translocates these molecules into the central pore of Clp P for degradation. In this study, we use evanescent nanometry/Electromagnetic tweezers to observe translocation activity of Clp X and degradation of Clp P. The distant-dependent intensity decay of evanescent wave was calibrated using Atomic Force Microscope. Vertical motions of a fluorescent bead were then converted into displacement by measured evanescent wave transfer function. This experiment reveals the fast, combinational unfolding and translocation activity of Clp XP under low force regime ($<80\text{pN}$) with the translocation size of 11-15nm. This study anticipates other AAA+ (ATP associated with a various cellular activities) protease to share similar features with Clp XP.

Pin-Joe Ko: Biology, CC'14

Quantification of tip proteins in *S. pombe* using confocal fluorescence microscopy

In many unicellular and multicellular organisms, cell polarity is crucial to differentiation, proliferation and the morphology. In the fission yeast *Schizosaccharomyces pombe*, cell polarity is maintained by protein clusters at the tips of microtubule bundles that carry these proteins to the long ends of the rod-shaped cell. However, while these tip proteins have been identified and are well-studied, not much is known concerning how the proteins gather on the microtubule tips. Furthermore, these proteins have never been individually quantified. In this project, we used high-resolution, confocal fluorescence microscopy to visualize and quantify natively tagged proteins at the microtubule tips. Different *S. pombe* strains were created that would fluoresce each specific protein. In order to obtain a count of proteins on each tip, we imaged the cells and compared relative fluorescence at protein clusters with a previously quantified control protein. Preliminary results indicate that dozens to hundreds of proteins can exist on a single microtubule tip. Furthermore, we found a large spread in the numbers of proteins among individual tips. In addition, we found that microtubule length does not correlate with protein quantity. These results imply a high tolerance for variation in protein numbers, which raises the question of whether the stoichiometric relationships between different proteins play a bigger role than the absolute quantities of the proteins.

Nilay Kumar: Physics, CC'15

Baryons and baryonic matter in the 't Hooft model under the heavy quark limit

Studying the nuclei of atoms from a purely theoretical standpoint using the quantum field theory of the strong interaction, quantum chromodynamics (QCD), is generally intractable due to the long range strength of the strong force. Additionally, the well-known Monte Carlo numerical methods of lattice QCD suffer from numerical instabilities and thus cannot be used to study finite density nuclear matter. Consequently, it is useful to study limiting cases of QCD in which calculations becomes tractable in order to gain some intuition into nuclear matter. The 't Hooft model, studied in this work, considers QCD in 2 spacetime dimensions in an artificial world where the number of quark colors, N_c is large. Unfortunately, even this problem is intractable except using a recently developed numerical technique discussed below.

Thus we consider the regime in which the mass of the quarks, M_Q , is large, as it allows us greater theoretical control.

First, we consider a baryon - in this artificial world, baryons consist of N_c quarks in a color-singlet interacting with each other through color-Coulomb interactions. In this regime of QCD, baryons can be described using a mean-field approximation. We used a variational approach to determine the baryon mass in terms of M_Q , N_c and the strong coupling constant. The mean-field approach used for the single baryon is assumed to hold for the multiple baryon sector of our model as well. It is shown that, at low densities, all leading-order interactions are repulsive, and an expression is determined for the energy per baryon.

We previously conducted a study of baryons and baryonic matter in the full 4 spacetime dimensions – one may ask the relevance of our 2 dimensional calculation. In fact, due to recent orbifold-inspired computational techniques, the 2 dimensional problem can be solved numerically. We hope that checking the results obtained here against numerical calculations will validate our (and previously, Witten's) assumption that the mean-field approximation does indeed hold in the many-baryon sector of both the 2 and 4 dimensional problems.

Alexis Kurmis: Chemistry, CC'13

Development of Enantioselective Reductive Coupling Reactions

Two key goals of modern organic synthesis are the synthesis of new C-C bonds from readily available starting materials and the formation of these bonds in an enantioselective manner. Advancements in these areas enable advancements in everything from materials chemistry to the development of new pharmaceutical agents. The vast majority of reactions currently used rely upon organometallic reagents, which require extra steps to synthesize and which can limit compatibility with many functional groups.

The goal of this summer was to optimize a reductive coupling reaction, which would eliminate the need for organometallics. All reaction parameters were investigated, including catalyst, temperature, solvent, substrates, reducing agent, and ligand. Both reactivity and enantioselectivity need to be high for a reaction to be considered successful. By the end of the summer, there were no conditions that met both these requirements, but some promising results were obtained.

With more development, this method could become an alternative to traditional reactions, where the use of organometallic reagents limits substrate scope. With a larger substrate scope, this reaction will be extremely useful in the synthesis of larger molecules.

Andre Lazar: Biology, CC'12

Modeling Integrin Clustering as Diffusion to a Sink

Cell motility is a vital cell function that depends on a cross-linked cytoskeletal actin network that involves numerous protein systems that coordinate signal and force transduction throughout the cell. Integrins are intermembrane proteins that link the extracellular matrix to the cytoskeleton through the formation of focal adhesions, diverse protein complexes that dynamically assemble and disassemble. Modeling focal adhesion growth and decay is therefore important in understanding cell motility at the molecular level. We examine the growth cycles of integrin clustering in focal adhesions and model their movement as

diffusion to a sink on the cell membrane. We show that early integrin clustering can be modeled as diffusion to a sink and that later stage clustering is accelerated due to myosin activity.

Dan Margulies: Chemical Physics, CC'13

A Tight Binding Model for Molecular Conductance and Transmission

Trends in computer technology show exponential growth in the number of components per integrated circuit. For this trend to continue, components must reach the molecular scale. Conventional electronics deals with current across macroscopic components. Molecular electronics studies the same principles in single molecules. Quantum mechanical models for electron dynamics guide and explain conductance experiments. Green's functions provide the theoretical framework for studying electron transport at these scales. Tight binding simplifies the calculations involved by considering only discrete sites, reframing electron transport as a matrix equation. Thus, any molecular junction can be described by a finite matrix.

I developed a computer program using NumPy (numerical python) to calculate the transmission of incident electrons through molecular junctions at a range of energies. Molecules were considered as Hamiltonian matrices, built using only nearest neighbor coupling and on-site energies. The molecules modeled included benzene, ethene, 1,3,5-hexatriene, and the conjugated infinitely long chain limit.

Transmission maxima are found to correlate with the energies of molecular orbitals, calculated using the same tight-binding model. Intuitively, this suggests that the molecular orbitals serve as conducting channels for incident electrons. This tight-binding model suggests that such a simple model is sufficient to derive useful qualitative predictions. Future research should expand the model to better explain the differences between transmission minima, of which there are several types.

James Nugent: Computer Science-Mathematics, CC'13

Compactification on Calabi Yau Manifolds

Superstring theory predicts six additional spatial dimensions in addition to the three dimensions of space and one of time we are familiar with. Assuming string theory is correct, the extra dimensions provide a means of unifying the four known fundamental interactions of physics, the Strong Nuclear, Weak Nuclear, Electromagnetism, and Gravitation. However, since we do not interact with these dimensions in our macroscopic life, a theoretical approach is necessary to explain why we do not see them. The most standard approach is to compactify them, or make them very small. While there are many shapes that these compactified dimensions could take, the primary candidate is a class of manifolds called a Calabi Yau manifold.

With the help of Dr. David Kagan of Columbia University, we are developing computational techniques to analyze fourteen such Calabi Yau Manifolds that are reasonable candidates for compactified space. These fourteen manifolds are chosen because they allow for a direct, hands-on set of examples for studying the physics of giving fundamental particles a large mass. Using Mathematica, algorithms for modelling the geometry of these Calabi Yaus were developed using Meijer G functions and Hypergeometric functions. They were then revised to maximize both accuracy and processing time. Graphs and data tables of the Meijer G functions were generated and refined to ensure accuracy. The Meijer G data was then used to generate data about the potentials whose minima indicate the possible compactifications of six-dimensional

space. These general algorithms could then be used to explore some of the physics involved in introducing large masses for the parameter field controlling certain geometrical aspects of the Calabi-Yau.

Julia Oktawiec: Chemistry, CC'13

Synthesis of a Organoboron Compound and Possible Novel Ligand

Since their discovery by Trofimenko, tris(pyrazolyl)hydroborato ("Tp") ligands and their derivatives have proven to be extremely versatile, capable of being adapted in various ways and used in various inorganic systems. Tp and related scorpionate ligands generally consist of a psuedo-tetrahedral boron atom, bonded to a hydrogen atom and three heterocycles that subsequently bind in a Lewis-base fashion (L_2X) to a metal atom. A variety of heterocycles have been used, some incorporating bulky substituents coupled to the heterocycles, and the boron atom may also be substituted. The versatility and tunability of scorpionate ligands have made them ubiquitous in inorganic chemistry, and have proven to be very useful, for example, as catalysts for organic transformations and polymerizations and as models for metalloenzymes, among other uses. In this project, a neutral borane ligand, $B(Mim^{Me})_3$, analogous to the anionic tris(2-mercapto-1-R-imidazolyl)hydroborato ligand, $HB(Mim^R)_3$ or (Tm^R) , has been targeted. The synthesis of the precursor compound, $Me_3PB(Mim^{Me})_3$ has been accomplished by treatment of trimethylphosphine-borane with three equivalents of 2-mercapto-1-methylimidazole ($Hmim^{Me}$). The product was characterized by homo and heteronuclear NMR spectroscopies, which provided evidence for the formation of $Me_3PB(Mim^{Me})_3$. Several reactions have been performed to use $Me_3PB(Mim^{Me})_3$ as a precursor for a $B(Mim^{Me})_3$ ligand, which we expect to bind as a tetradentate ligand (L_3Z) to form complexes known as boratranes. Unfortunately, to date, no structurally characterized metal complexes with a $B(Mim^{Me})_3$ ligand have been obtained, but evidence for their formation has been observed.

Darpan Patel: Biology, CC'14

Iron-Dependent, Non-Apoptotic Cancer Cell Death Requires NADPH Oxidase (NOX) Enzyme Activity

Treatment of cancer cells *in vitro* with the small molecule erastin induces non-apoptotic, iron-dependent cell death. Notably, this process involves increased production of reactive oxygen species (ROS). The NADPH oxidase (NOX) family of enzymes, a key source of intracellular ROS, was analyzed to gain insights into the mechanism of action of erastin. A two-pronged approach was used to determine the necessity of NOX activity for erastin-induced death: (1) NOX inhibitor profiling of erastin versus other anti-cancer drugs, and (2) silencing of NOX-related genes using RNA interference (RNAi). Cancer cells were rescued from erastin-induced death by small molecules 2-acetylphenothiazine (2-APT) and GKT137831, both of which are selective inhibitors of the NOX1 isoform. Silencing of NOX1 gene expression protected cells from erastin-induced death, while silencing of the other NOX isoforms (2-5) did not yield appreciable rescue. This is consistent with the small molecule data, and together they suggest NOX1 might be responsible for increased ROS generation seen in erastin-induced death. A better understanding of NOX-dependent, non-apoptotic form of cell death could aid deployment of new small molecule drugs, such as erastin, to circumvent issues with acquired cancer cell resistance to apoptosis.

Milesh Patel: Biochemistry, CC'12

Barriers to Optimal Nutrition for Very Low Birthweight Infants: A Quality Improvement Study on Parenteral Amino Acid Administration

Advances in perinatal and neonatal care have increased the survival of preterm infants. However, improving the long-term outcomes of these surviving infants remains a challenge. Compared to normal fetuses of the same gestational age, the postnatal growth of premature infants is restricted. The discrepancy between extrauterine and intrauterine growth at the same gestational age has been attributed to protein and energy deficits. This is particularly important because poor neurological outcomes and pulmonary morbidity have been associated with delayed postnatal growth.

In response to these new findings, the Neonatal Intensive Care Unit at Children's Hospital Boston has updated its guidelines for administering parenteral nutrition (PN). A retrospective chart review revealed that these guidelines were not being met, with less than a third adherent on day 2. In most cases no barrier could be identified. This study is a prospective patient-oriented quality improvement project that incorporates the practitioner's perspective. For each patient admitted to the NICU, we monitored IV fluid and PN orders for adherence each day for 3 days. If an order was not adherent, we asked the prescriber to choose from a list of potential reasons, or to provide another reason. We also monitored each patient's BUN level for toxicity.

The major barrier on day 1 was receiving starter PN off-hours. We found that some practitioners were not aware of the availability or indication for starter PN. In addition, there were misconceptions about PN administration in general. We looked specifically to make changes to our process to improve our outcome. Because we found that the indication for starter PN in the CHAMPS software is obtuse, we can change the process by which starter PN is ordered, making it easier and more intuitive. In addition, we can modify practitioner training to specifically address misconceptions about PN administration. Knowledge deficits and logistical problems can be addressed directly in the context of an ongoing quality improvement project, leading to improvements in adherence, and ultimately nutrition-related outcomes for these patients.

Jenny Shao: Biochemistry, CC'13

Investigating the Role of Actin Polymerization State in Synaptic Plasticity

A critical component of the cytoskeleton and ubiquitous in eukaryotes, actin has been implicated in several important functions in learning and memory. This long-term endeavor strives to identify the relationship between the actin polymerization state—the dynamic equilibrium between g-actin and f-actin—and the local synaptic strength, which thereby sheds light on actin's function in the broader phenomenon of learning. To accomplish these aims, it is necessary to first develop visualization system that provides an accurate, dynamic, and high-resolution representation of the polymerization state: we utilized a variation of Forster Resonance Energy Transfer (FRET), namely energy-migration FRET (emFRET or homoFRET). Since a single fluorophore is used in emFRET, the method eliminates potential noise from fluorophore crosstalk and combinatorial issues that are often observed in regular FRET. Since quantitative analyses demonstrated that mStrawberry had the optimal optical properties, most importantly low levels of Rayleigh Scattering, it was selected to visualize actin dynamics in tissue. Molecular cloning was then utilized to generate an mStrawberry-Actin vector. Specifically, after obtaining pmStrawberry and pActin-

GFP vectors from Clontech, the region corresponding to the fluorophore (mStrawberry) was amplified via PCR, the inserts and vector were purified, and the inserts were ligated into the actin backbone. Restriction enzyme digestion and gel electrophoresis analyses subsequently indicated that the cloning and ligation processes were successful. Bacterial transformation and Maxipreps were then used to harvest the newly generated DNA (Actin-mStrawberry). To confirm the efficacy of the Actin-mStrawberry plasmid, the DNA was transfected into HEK cells; robust expression levels that were detected after 24 hours indicated that the newly constructed plasmid did indeed contain mStrawberry and actin in the correct sequence. Furthermore, DNA sequencing also returned a 100% match between the expected and actual plasmid sequence. This construct, once injected into either culture or mouse, gives rise to a precise and high-resolution representation of actin dynamics. By shedding light on the role of actin in learning and memory, this study also informs us on possible mechanisms of several pathological conditions, such as Alzheimer's and Huntington's diseases, in which clear distortions in learning and memory are observed.

Katharina Shaw: Chemistry, CC'13

Synthesis of Resveratrol-Derived Analogues: Phosphorylated Isopaucifloral F, Phosphorylated Paucifloral F, and Yuccaone A

For the past decade, resveratrol – a ubiquitous, polyphenolic phytoalexin found in grape skins and red wine – has captivated the attention of the scientific community. In addition to its potent antifungal, anti-aging, and neuroprotective properties, resveratrol has been cited as responsible for the “French paradox” – a concept formulated by epidemiologists to describe the low incidence of coronary heart disease in French people despite their high intakes of cholesterol and saturated fats.¹ However, while much attention continues to be devoted to resveratrol, its analogues have been largely disregarded in spite of their vast clinical potential. The difficulties posed by their synthesis, coupled with the inability to isolate sufficient quantities from natural sources, have rendered many such oligomers unattainable. Thus, for this project, the controlled and potentially scalable synthesis of three such oligomers was undertaken – namely, that of phosphorylated Paucifloral F, phosphorylated Isopaucifloral F, and Yuccaone A. Previous attempts to biomimetically access such members of the resveratrol family have proven unsuccessful – even in those cases where the desired resveratrol derivative was obtained, an array of non-natural products were generated.² As a result, the synthetic approach utilized here rejected a biomimetic pathway in favor of reagent-guided functionalization of a unique core molecule that possessed multiple sites of similar reactivity. Using a three-aryl ring precursor as the core building block, both phosphorylated Paucifloral F and Isopaucifloral F could be generated in relatively high yield. Careful manipulation of the same triaryl precursor remains underway for the synthesis of Yuccaone A. In light of resveratrol's promising array of biochemical behaviors, the controlled syntheses of oligomers such as these may be key to tapping the full clinical potential of this family of natural products.

Hyoun Ju Sohn: Physics, CC'13

Crystal formation of Dibenzotetrathienocoronenes (DBTTC) on graphite in ambient scanning tunneling microscopy (STM) using platinum-iridium tips

We investigate the use of graphene surfaces to assemble organic molecules into crystals. The morphology of such crystals is important in applications such as solar cells. We choose the Dibenzotetrathienocoronenes molecule since it has optical response and has a pi backbone that can interact with the graphene surface. Crystals were formed by drop-casting from a solution of DBTTC in high vacuum and the morphology of the films was studied using scanning tunneling microscopy (STM). Initial STM analysis was done on graphite and graphene using platinum-iridium tips to find optimal conditions, ranging bias (-1.0~ 1.0V) and setpoint (500pA~2nA). The size of the scan was reduced from 100nm to as low as 5nm while generally maintaining scan rates of 5~10Hz for graphite and 2~5Hz for graphene. The DBTTC sample that was aimed to deposit a 10~15nm film on graphite were seen to form aligned stalk-like structures on the substrate with roughly 10nm heights for alignments with 250nm widths. In the sparser regions, hook-shaped 50 x 50nm stalks captured the crystal forming process that involves growing uniformly flat layers of DBTTC between the converging stalks as the deposition progressed. A difference in periodicity is also observed between a graphite surface and a thin DBTTC surface(single to few layers thick) on graphite. Future experiments will focus on the study of a single atomic layer of DBTTC on graphite and graphene.

Tyler St. Denis: Biochemistry, CC'15

Enhancement of Antimicrobial Photodynamic Therapy by Potassium Thiocyanate/ Selenocyanate Salts

The emergence of antibiotic-resistant pathogens has initiated global searches for new antimicrobial modalities. Photodynamic therapy (PDT) is a novel antimicrobial technique consisting of visible-light, a light sensitive dye, and oxygen, which together yield reactive oxygen species (ROS). ROS reactivity is diffusion rate controlled and is thus limited to the cellular envelope of bacteria. In efforts to potentiate bactericidal activity of PDT, this report sought to create less reactive, but longer-lived radical species, capable of deeply penetrating bacteria. Comparing a control PDT regimen to PDT with the pseudohalide salts thiocyanate (SCN^-) or selenocyanate (SeCN^-), PDT-mediated killing of the Gram-negative *Escherichia coli* and the Gram-positive *Staphylococcus aureus* was potentiated by 1-4 \log_{10} with the addition of SCN^- / SeCN^- . This is presumed to be the result of the formation of SCN^- / SeCN^- radicals, likely due to reactivity of SCN^- / SeCN^- with the hydroxyl radical (OH^\bullet). Pseudohalide radical formation was confirmed by theoretical redox potential studies and comparison of the bactericidal effect of a chemical OH^\bullet generator (Fenton's reagent) with or without SCN^- / SeCN^- . Interestingly, potentiation of PDT was not additive and at high concentrations, SCN^- and SeCN^- reduced PDT killing, presumably due to the formation of insoluble methylene blue-pseudohalide salt products.

Scott Zhang: Astrophysics, CC'14

Diffuse high-energy neutrino spectra from high and low-luminosity gamma-ray bursts

The fully operating IceCube neutrino observatory, designed to detect TeV-scale high energy neutrinos, opens up a new window for high energy astrophysics. Gamma Ray Bursts (GRBs), with their extreme energetics, are one of the most plausible sources of diffuse high energy neutrinos detectable by IceCube. While some, high-luminosity (HL) GRBs are individually much brighter than many other, low-luminosity (LL) GRBs, the latter subclass may play a major role in contributing to the diffuse high-energy neutrino background, due to their much higher abundance, as well as their somewhat different emission process. Further, LL-GRBs may be the key in understanding choked GRBs, an important subclass of GRBs with no observable gamma-ray emission. It is important to compare the contribution of diffuse high energy neutrinos by both high-luminosity (HL) and low-luminosity (LL) GRBs. Using the gamma ray data of GRBs collected by the Swift satellite, assuming the neutrino spectrum for individual GRB derived by Guetta et al. and the rate of HL and LL GRB per year estimated by Liang et al., I calculated the total diffuse neutrino spectrum by both HL and LL-GRBs. My result is consistent with the neutrino spectrum 90% CL upper limit implied by cosmic ray observation (Ahlers et. al. 2011) except for the neutrino energy range $6e6 \sim 7e7$ GeV, but it suggests that HL GRBs typically produce 1~2 orders of magnitude more neutrino than LL GRBs, contrary to the claim of some authors that the neutrino spectrum by HL and LL-GRBs are comparable. This may be because the emission mechanism in LL-GRBs differ from the Guetta et al. emission model due to, e.g., the larger abundance of baryons in the jet.
