This issue of the

Caltech Undergraduate Research
Journal highlights the exceptional
research of three young scholars:
Christina Daniel, Edward Huang, and
Patrick Yu; and features interviews
with two Caltech faculty members:
Jonas Peters, Professor of Chemistry,
and Doris Tsao, Professor of Biology.





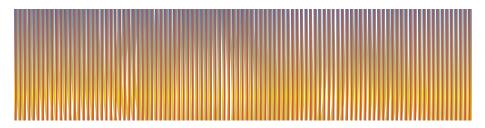
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by Patrick Yu

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This fall marks the end of yet another summer of intense undergraduate research at Caltech and JPL. Every year, hundreds of students from around the country and the globe are drawn to Pasadena for ten weeks of research under the leadership of talented faculty mentors. Through the guidance of these dedicated mentors, as well as the tireless efforts of Caltech's Student Faculty Programs office, these students have been able to take their first steps of what will become a long journey of scientific curiosity and discovery.

This issue of the Caltech Undergraduate Research Journal highlights the exceptional research of three young scholars: Christina Daniel, Edward Huang, and Patrick Yu. With topics ranging from novel information retrieval algorithms to new materials for high-efficiency solar cells, these three articles exemplify the great diversity of work currently being performed by undergraduate students.

In this issue, CURJ is pleased to feature interviews with two Caltech faculty members: Jonas Peters, Professor of Chemistry, and Doris Tsao, Professor of Biology. The accomplishments of both professors, as well as their enthusiasm and dedication to pushing the limits of science, serve as an inspiration to all young scientists at Caltech.

We encourage you to visit our website at curj.caltech.edu, where you can find past CURJ issues and more information about the journal. We welcome your comments and feedback. Thank you for picking up this latest issue!

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Best regards,

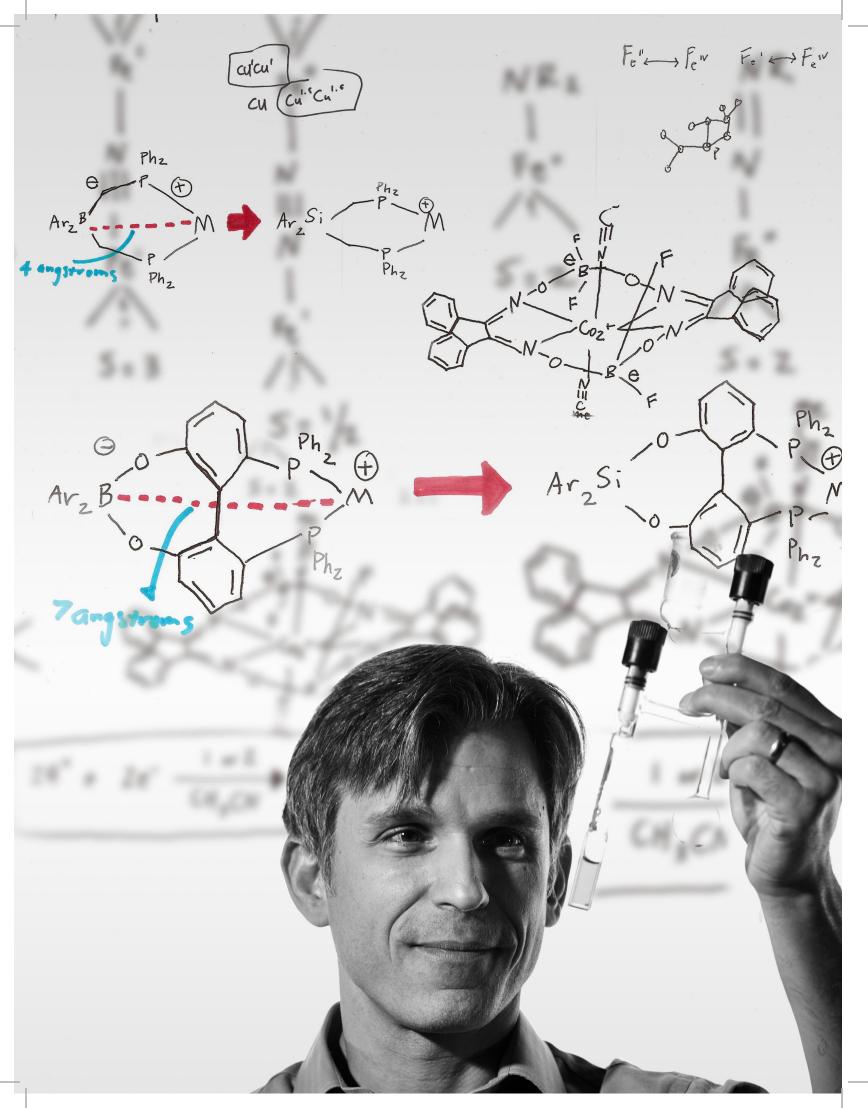
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Caltech Undergraduate Research Journal

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interview Professor Jonas Peters

What does your lab work on?

My lab is a synthetic inorganic lab, which means that we make fundamentally new coordination complexes. The types of compounds we make are interesting structures in and of themselves from the perspective of electronic structure and bonding. Sometimes these complexes push the boundaries of what we think might be stable or unstable. The backdrop of most of the projects we work on concerns multi-electron redox reactions of small molecules, transformations that are essential to life.

What sorts of applications does your research have?

We ultimately hope to use our expertise in synthesis, spectroscopy, and mechanism to discover catalytic transformations relevant to sustainable fuel and food. One of the great challenges of chemistry in terms of societal needs is to learn how to synthetically couple sunlight to drive important transformations. Such transformations include, for instance, fixing carbon to make fuel (as in photosynthesis), or nitrogen to make fertilizer (as in nitrogen fixation). These are energy-intensive transformations that can be coupled with water oxidation and powered by sunlight. One of the core research areas of our lab is the study of ironmediated nitrogen fixation. 3.5 billion people on the planet are fed by fertilizer made by the Haber-Bosch process, which turns nitrogen gas from the atmosphere into ammonia. We hope that there's ultimately a more sustainable way than the Haber-Bosch process to make ammonia; nature has figured out a way, and we hope chemists can too. In addition, we investigate reactions relevant to storing fuel via sunlight and energy conversion such as hydrogen evolution and carbon dioxide fixation. We also collaborate with Professor Greg Fu's lab to use light and transition metal complexes to induce cross-coupling reactions relevant to organic methodology development.

What do you find most exciting about your research?

When we're studying some kind of unusual reaction, we initially feel like we're wandering around blindly in the dark. But based on experiments, literature, and talking to people, we eventually start to piece the chemical puzzle together to gain a better understanding of how things are working. I find it most exciting when we have that initial spark of understanding of an unusual transformation that sets the stage for lots of experiments to develop it further. Ultimately, I want us to keep working on problems that stimulate our intellectual interest and to keep discovering new approaches for catalysis in the diverse areas of catalysis we work in. I also hope that our research enables students to get excited about chemistry, inorganic chemistry in particular.

How did you get started in your field?

As an undergrad at UChicago, I initially figured I would be a biology major, so I was taking classes in both biology and chemistry. I thought that if I had a good foundation in chemistry, I could branch into biology. I worked in a cell biology lab as a freshman, and the next year I decided to join a pure chemistry lab to get a new experience. I found that lab to be such a fun playground that I remained there for several years.

My mentor was Professor Gregory L. Hillhouse, who passed away of cancer in 2014. He was a wonderfully devoted undergraduate mentor and friend. He had a way of making the research a heck of a lot more fun than it would have been without him. He also impressed upon me that if I was willing to make the effort, the field would reciprocate by providing a career path for me. I didn't initially have the confidence to go into the field of chemistry, but he helped me realize that I had the necessary ingredients to succeed and that it would be worth my while.

What advice do you have for Caltech students?

Definitely take fewer classes and spend more time doing research in a lab during the academic year. You will remember and be rewarded by lab work much more than taking classes. I wish I could change Caltech students' habit of enrolling in too many time-consuming classes and, frankly, not getting what they should out of those classes because they stretch themselves too thin. A lot of my colleagues share this opinion. I also think it's important to remember to keep it fun while you're an undergraduate. Science should be fun, though sometimes it gets a little serious and maybe a little monotonous. We have to remind ourselves of that as we go through our careers, but at the end of the day science is both important and fun. I think that undergrads should keep this message in mind and occasionally remind their research advisers of it too!

What hobbies and interests do you have?

I love sports like softball and touch football, and especially baseball. There's no place I'd rather be than on a baseball field. But I'm awful at basketball, and also pretty lousy at soccer. Niles Pierce is trying to fix my soccer deficiency. He just helped me to buy my first pair of soccer cleats, and has been telling me that because I can still run at my age I have a chance to play decently "in my age group." I also enjoy activities like jogging, hiking, skiing, and camping. I love to garden and cook at home, and when I can focus, I really like to read fictional literature.





interview Professor Doris Tsao

"...the brain transforms the retinal input, which is an array of pixels, into a representation of visual objects..."

Many students would be interested to know about your current research, summarize what your lab is working on?

The big question my lab is interested in is how the brain represents visual objects. We are studying this in two species: macaque monkeys, because their visual system is very similar to that of humans, and mice, because there is a wide variety of techniques we can use to study neural circuits in mice. We are using multiple approaches in both species: in monkeys, we use fMRI (functional magnetic resonance imaging), which gives a big picture of how the brain is organized by measuring blood flow across the entire brain in response to different visual stimuli. We also use single unit recording, which lets us record electrical activity from single neurons in regions of interest that we identify using fMRI.

In essence, we are trying to understand the computational principles by which the brain transforms the retinal input, which is an array of pixels, into a representation of visual objects in space. We've done a lot of work on understanding face processing, and found out that the brain contains six patches of cortex in each hemisphere that are specialized for processing faces. This creates an intriguing biological problem of figuring out what happens in each of the six patches.

While we think that monkeys see the world very much like we do, we are at a much earlier stage in our investigation of the

mouse visual system because we currently don't know what mice see. We're testing through behavioral experiments whether mice perceive whole objects, that is, whether they can perceive units that are bound together. We are also using state-of-the-art two-photon imaging, electrophysiological techniques, anatomical tracing and optogenetics to understand the neural mechanism for object perception, if mice can indeed perceive objects.

Could you tell us more about the behavioral experiments in mice? How do you test whether mice can perceive whole objects?

We have designed a task in which mice have to distinguish between letters X and H. For humans, if the letters are partially occluded, we can still distinguish them clearly, even with a complicated pattern of occlusion.

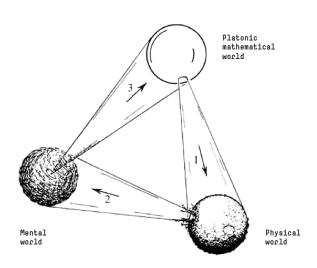
This is a computation we make effortlessly because we can see objects despite occlusion, and we will test whether mice can distinguish the letters the same way as us.

What was your main motivation to pursue neuroscience?

My motivation came from the realization that we could understand space by recording from neurons. I've always been interested in geometry, and the fact that our brain can represent infinite space with a finite set of neurons seems remarkable to me. That was the motivation I had back in high school and I'm

"Our consciousness is part of the physical world, the mathematical world is conceived by our consciousness, and all of physics is described by mathematics."

happy to say that I'm studying the same problem that has been fascinating me ever since. In high school, I came across the book "Shadows of the Mind" by Roger Penrose. I remember a beautiful figure in the book of the impossible triangle, with its three vertices being the physical world, the platonic mathematical world, and our subjective world of consciousness. Our consciousness is part of the physical world, the mathematical world is conceived by our consciousness, and all of physics is described by mathematics. There is an underlying unity to these three different ways of looking at reality. The great thing about neuroscience is that we don't have to see this impossible triangle as a mystical entity, but we can perform experiments and really try to understand these connections. We can understand how the brain arises from physical neurons, as well as how mathematical percepts arise from computations in the brain. [see figure below]



You also studied math as an undergrad at Caltech. How has math contributed to your understanding of the visual system?

I think the visual system is essentially a cortical geometric engine. The computations of neurons in the visual cortex are creating our perception of space: when we look at the world, the visual system is continuously measuring the shapes of object surfaces, their distances and spatial relationship to each other, and doing an elaborate, geometric computation which actually produces a conscious percept of these mathematical objects. Unfortunately, we currently have very little understanding of these processes.

How has our understanding of vision progressed in recent years?

I think we are still in very early days. We have a coarse understanding of how the visual system is organized overall. We know about a few interesting visual areas, but we are lacking a deep understanding of what is precisely computed in each area and how these representations can be accessed by our consciousness. We should not be depressed by this, however, because the first electrophysiological studies of the visual system only happened less than a hundred years ago. If we look at physics, it took about 200 years to get from Newton to Maxwell, and that's just Phys 1.

So you were an undergrad at Caltech. How does it feel being back here? What are the major changes that you have observed?

I feel like the undergrads have to follow a few more rules. You guys don't have the south master anymore, to get access to any



building you want. There are certain things that haven't changed, though. The thing that I loved the most about being an undergrad here was the core curriculum, which required us to take courses in a wide variety of disciplines. After I went through the experience, the whole university was like my playground - I felt that I could master any subject if I put enough effort, and no subject was out of bounds because I was a biology major. Talking to the undergrads today, I feel like they are still interested in many different subjects in the same way, and the spirit of the place is exactly the same.

What aspect of being a researcher do you enjoy the most?

I love the fact that I'm working to answer the questions that I really want to know the answers to. Most days I get up, go to work, go home, go to sleep, and then repeat. Once in a blue moon, I think, this is so weird. Why do I exist? How can I be conscious? Why does the world appear the way it does? And on those blue moons, I thank my lucky stars that I'm a neuroscientist, and I get to make my living digging my way out of this confusion. There are a lot of difficulties stemming from the social aspect of science (maintaining funding and dealing with reviewers), but essentially I am completely independent, I am free to choose to study the things that I'm curious about and I don't have to work for anyone else. I love to work with incredibly smart and motivated young people every day. When we make a discovery, the feeling is amazing—but that's just the vista point before the climb continues. What are your views on the future of neuroscience research? Do you think the visual system can be decoded in the near future? So many new techniques have emerged over the past decade, and the next big challenge is to apply these techniques to discover fundamental new principles

about the brain. Right now, I feel that our conceptual framework for understanding how the brain works is still very limited. I do think that it's possible to completely decode vision. Our percept of surrounding objects is completely deterministic. The visual system is a machine that is sitting there for us to probe as deeply as we want, and we should ultimately be able to figure out how it works.

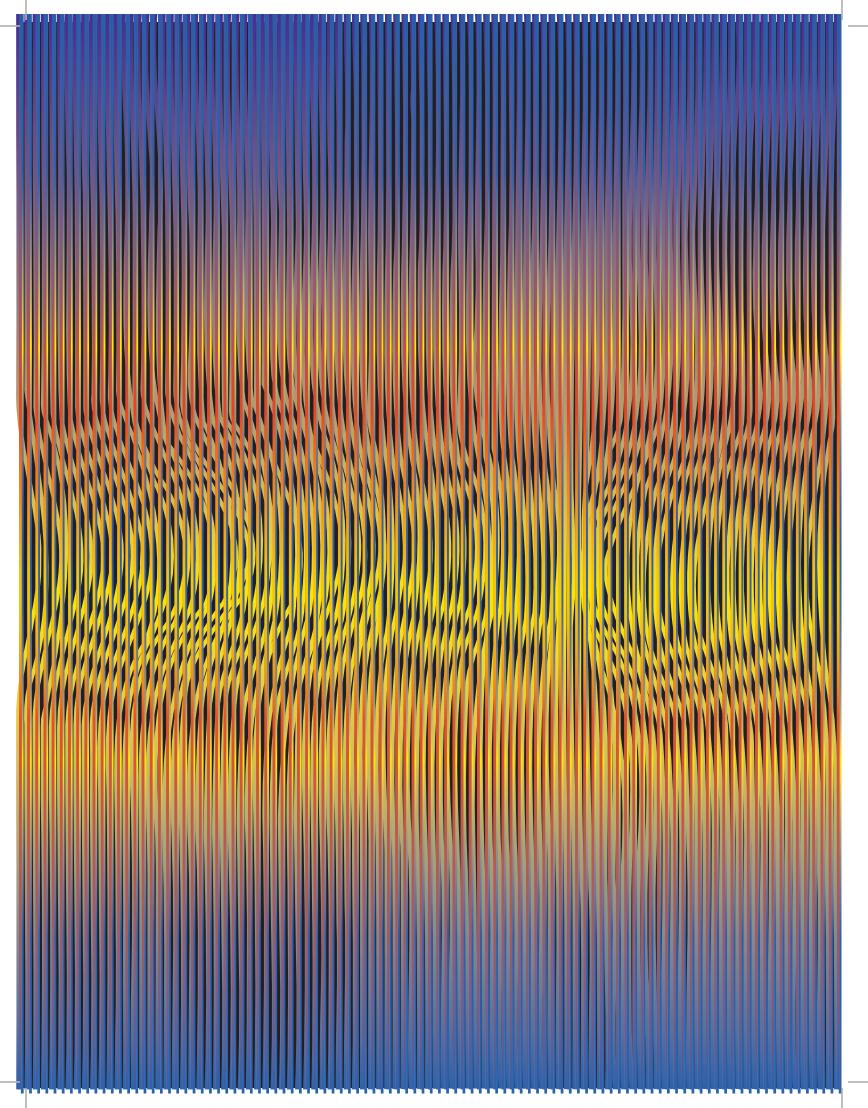
What are your views on the future of neuroscience research? Do you think the visual system can be decoded in the near future?

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I do think that it's possible to completely decode vision. Our percept of surrounding objects is completely deterministic. The visual system is a machine that is sitting there for us to probe as deeply as we want, and we should ultimately be able to figure out how it works.

What advice do you have for undergrads who are planning to go into research, and more specifically into neuroscience research?

I think you should follow your curiosity in a completely sincere way and not worry at all about what is trending right now. Just delve into subjects that really interest you and do what you really like.



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article

Magnetism and Advanced LIGO

author Christina Daniel



biography

Hometown: Santa Barbara College: UCLA Major: Aerospace Engineering

Year: 3rd Hobbies: classical piano, reading

"Detection of gravitational waves is encoded in the behavior of the recombined laser light."

THE MOTIVATION

LIGO, the Laser Interferometer Gravitational-Wave Observatory, is a physics experiment that aims to directly detect a gravitational wave, an unconfirmed component of Albert Einstein's theory of general relativity. LIGO is composed of two detectors called interferometers; one of which is in Hanford, Washington, and the other in Livingston, Louisiana. A LIGO interferometer consists of two perpendicular, four kilometer arms. At the end of each arm is a mirror, called a test mass. Normally, laser light splits into both arms, reflects off both test masses, and then recombines in the same phase. In theory, a gravitational wave stretches space along one arm and compresses space along another, which causes the laser light to travel different distances and recombine in different phases. Thus, detection of gravitational waves can be achieved by studying the behavior of the recombined laser light.

Environmental factors can affect the interferometer's measurements; thus, knowing how the environment affects the interferometer is crucial for unambiguous, accurate detection of a gravitational wave. LIGO uses a Physical Environment Monitoring (PEM) system to monitor each interferometer's surroundings. An important environmental factor is a magnetic field. The current carrying the gravitational wave signal runs through electromagnets to produce magnetic fields which move the test mass to its original position. Such movement is possible because tiny magnets are a part of the test mass suspension system. Therefore, an ambient magnetic field can displace a test mass, which would greatly affect the measurement of gravitational waves.

This paper addresses the progress made in monitoring magnetic fields around the Hanford interferometer (abbreviated LHO).

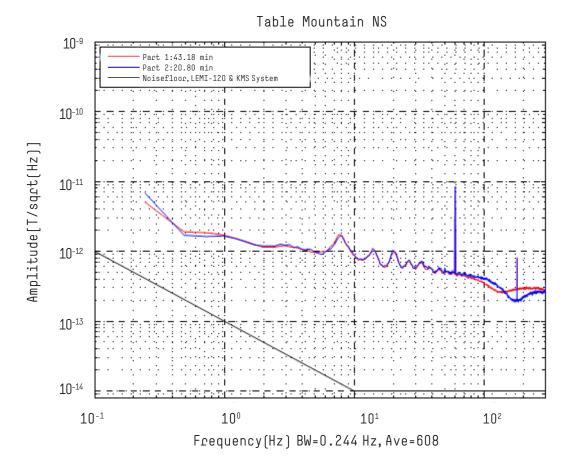


Figure 1: This plot reveals peaks due to Schumann Resonances at various frequencies. This magnetic field data was taken in a North-South orientation at Table Mountain, a sufficiently isolated location for recording low-amplitude magnetic fields.

The Research: Global Magnetic Fields

A global magnetic field, or a magnetic field detectable on the global scale, could potentially cause a signal that the interferometers would falsely detect as a gravitational wave. The current low end of the sensitivity range (range of confidence in detection) is 10 Hz. Thus, LIGO's interferometers are predicted to confidently detect gravitational waves varying at frequencies of 10 Hz. By monitoring global magnetic fields, we can increase the sensitivity of the detectors, by subtracting magnetic field data from gravitational wave data. Global magnetic fields have small amplitudes, so measuring them requires that a sensitive magnetometer be placed in the right location. This location needs to be magnetically isolated (minimally influenced by other magnetic fields). Magnetic field data was collected and analyzed from four locations.

For each location, we took two sets of data—one to measure the magnetic field along the North-South axis of Earth, the other to measure along the East-West axis. When taking global magnetic field data, we did not want to measure magnetic fields from power lines and other devices. In the United States, the standard currents in wires oscillate at 60 Hz. To see which location was the most magnetically isolated, we compared each site's magnetic field peak at 60 Hz. Table Mountain was found to be the best site, because its North-South and East-West data sets had the smallest peaks at 60 Hz, at approximately $101T/\sqrt{Hz}$ in magnitude.

The Table Mountain data revealed a source of a global magnetic field called a Schumann Resonance. A Schumann Resonance is caused by lightning, which produces an electrostatic discharge (a sudden flow of charges between two oppositely charged surfaces). This electrostatic discharge produces electromagnetic

waves which propagate spherically, resonating in a spherical cavity defined by the Earth's surface and the ionosphere. The resonant frequencies of the Schumann Resonance are spaced at intervals of approximately 6.5 Hz, with 7.83 Hz as the fundamental (lowest) frequency. Figures 1 and 2 show Schumann Resonance peaks at these frequencies.

The data acquisition system split the Table Mountain data into parts, which were combined in Matlab. The long data set revealed a low frequency magnetic field, since more time allowed for the presence of a longer wavelength, and thus a lower frequency. The low frequency magnetic field at approximately 0.01 Hz fell into a frequency band of ULF electromagnetic waves. In Figures 3 and 4, the peaks at approximately 0.01 Hz represent these ULF waves. However, since the frequency of the ULF waves range from 1 mHz to 1 Hz, which falls below the 10 Hz end of the Advanced LIGO sensitivity range, ULF waves are not of concern.

Local Magnetic Fields

A local magnetic field, or a magnetic field specific to one of the LIGO observatories, can also affect an interferometer's measurements. To measure ambient magnetic fields, LIGO uses Bartington fluxgate magnetometers around each interferometer. Each magnetometer sends an analog, or voltage, signal to the signal conditioning box, which sends the signal to a custom filter box. The signal is then converted into a digital signal, which can be displayed in a readable fashion on a computer screen. The custom filter boxes were modified so that the PEM magnetometers can provide accurate data at 10 Hz. Nine magnetometer filter boxes were modified. To modify the filter boxes, the crossover frequency, defined as:

$$f = \frac{1}{\Omega RC}$$

needed to be between 0.1 and 1 Hz, which was sufficiently below the desired sensitivity of 10 Hz. If the angular frequency w and capacitance C was kept constant, a crossover frequency of 0.6 Hz was obtained when changing the resistance R from 1 k Ω to 5 k Ω . However, the gain, or signal amplification in the circuit, must remain the same. We use :

$$Gain = \frac{R_2}{R_2}$$

The Gain of the circuit must remain 100; since R_1 is 5 k Ω , as defined from the crossover frequency calculation, R_{\circ} must be



500 k Ω . Therefore, modifying the filter boxes involved replacing 1 k Ω and 100 k Ω resistors with 5 k Ω and 500 k Ω resistors, respectively.

In addition to modifying the filter boxes, the mounting of several magnetometers was improved. A custom mount design was modified to allow for securing magnetometers to tripods. Also, one of the magnetometers was re-oriented vertically, which prevents the supporting ferromagnetic metal from disrupting the sensor's magnetic field measurements. In addition, the axes on certain magnetometers were relabeled to be aligned with the LIGO coordinate system.

Magnetic Field from Electronic Devices

In the event of a power loss while the interferometer is taking data, the APC Smart-UPS (Model: 1500, Max Configurable Power: 980 Watts/1440 VA) will continue powering the laser to prevent laser damage. The UPS draws a large amount of current;

thus, it was necessary to measure the device's magnetic field at various distances to determine how close the UPS could be to other equipment, including the interferometer. The maximum allowable magnetic field at 60 Hz from any electronic device was defined to be 0.4 nT, which is one tenth of the root mean square 60 Hz magnetic field during Initial LIGO science runs.

For magnetic measurements, we used two 500 Watt lights, a magnetometer, and the UPS. We determined that the UPS must be placed at its minimum distance whenever the device is plugged in, because its plugged-in while on and plugged-in while off configurations produced similar magnetic field magnitudes. At 1 meter, we measured the magnetic field at three different angles relative to the physical center of the device. We determined that the magnetic field was the strongest when aligned with the device's front left edge. The remaining measurements were taken at this angle. We took data from distances 3 to 39 feet, with a constant interval of 3 feet. At each distance,

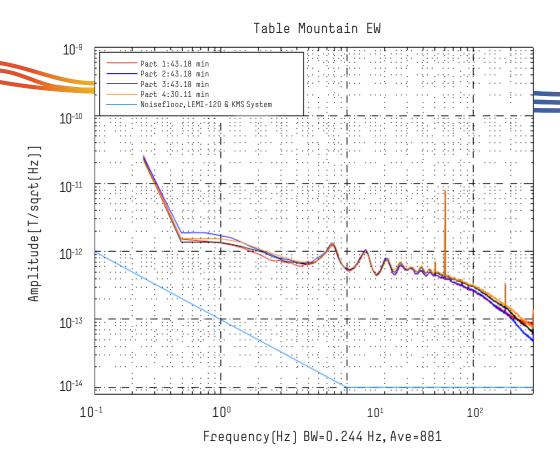


Figure 2: Similar to Figure 1, this plot reveals peaks due to Schumann Resonances at various frequencies. This magnetic field data was taken in an East-West orientation at Table Mountain.



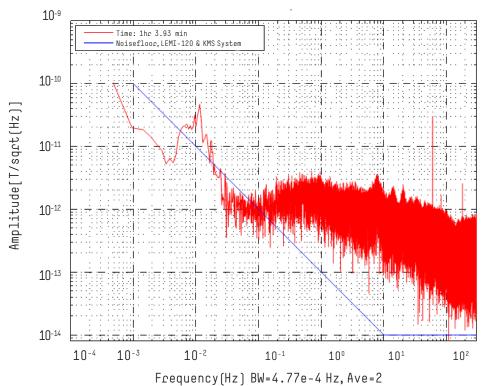


Figure 3: This plot reveals a peak at approximately 0.01 Hz due to an Ultra-Low Frequency wave, which is not of concern to Advanced LIGO. This magnetic field data was taken in a North-South orientation.

Table Mountain EW, Concatenated

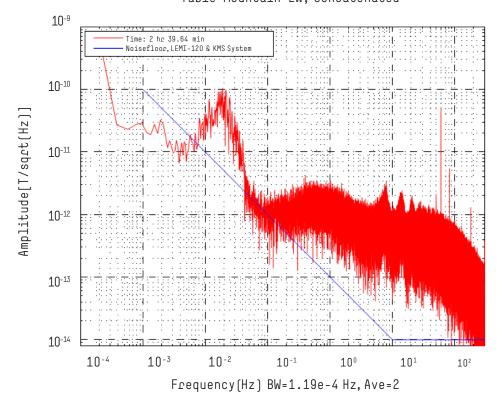


Figure 4: Similar to Figure 3, this plot reveals a peak at approximately 0.01 Hz due to an Ultra-Low Frequency wave, which is not of concern to Advanced LIGO. This magnetic field data was taken in an East-West orientation.

UPS Magnetic Field Attenuation Data Set 1

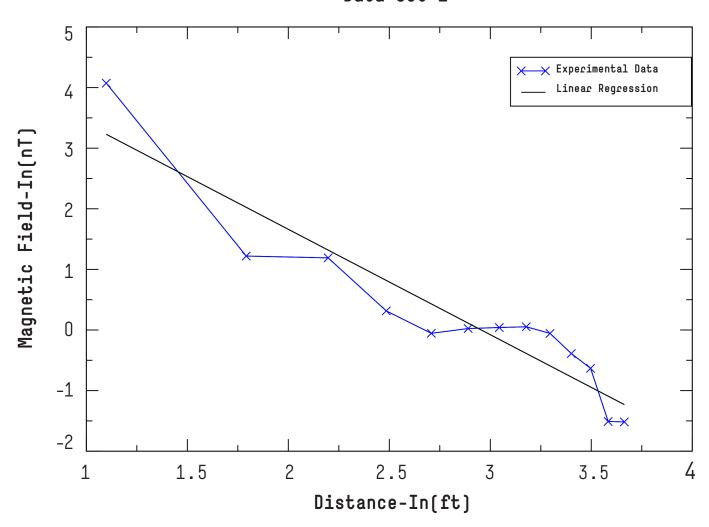


Figure 5: The fitted curve, shown in black, shows that the UPS system must be at least 33 feet away from other electronic devices, including the interferometer.

the power spectra of the magnetic field was recorded when the UPS was plugged in and unplugged. We used a program called Grace to perform linear regression on the data produced. We plotted the natural log of the magnetic field vs. the natural log of the distance, and got a fitted curve:

$B = 171d^{-1.74}$

thus, when y is 0.4 nT (maximum allowable field), must be 33 ft, which is the minimum distance the UPS must be away from other electronic equipment at the Hanford site. Figure 5 shows the magnetic field attenuation and linear regression.

The Next Step:

Future work could investigate magnetic coupling to the gravitational wave channel. Quantifying magnetic coupling to the gravitational wave channel would involve figuring out how many Tesla is required to move a test mass one meter. Further study should look at how magnetic fields affect other PEM sensors, such as seismometers. In addition, a magnetometer can be calibrated by imposing a known magnetic field through one axis of the magnetometer. A solenoid would be used to produce the known magnetic field, which can be compared to the measurements reported by the magnetometer.



"Further study should look at how magnetic fields affect other PEM sensors, such as seismometers."



- 1. E.Thrane, N. Christensen, R. M. S. Schofield. Correlated Magnetic Noise in Global Networks of Gravitational-wave Interferometers: Observations and Implications.
- 2. Robert L. McPherron. Magnetic Pulsations: Their Sources and Relation to Solar Wind and Geomagnetic Activity.
- 3. Joshua Myers. Magnetometer Whitening Filter. LIGO, DCC number D070443.

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article

Development and Analysis of Intuitive Information Retrieval

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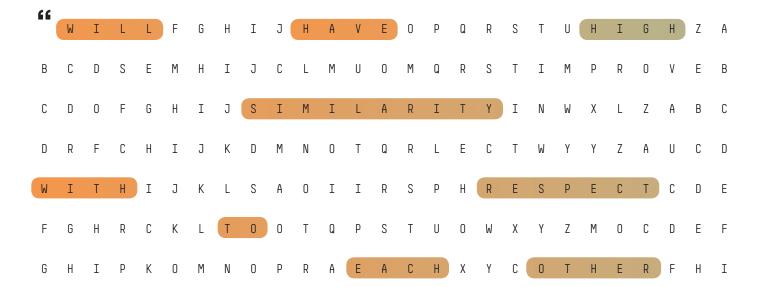
Edward Huang

Jehoshua Bruck & Farzad Farnoud

"Many search algorithms look exclusively for keywords."

ABSTRACT

Collections of data can be so large that traditional techniques of information retrieval and processing are impractical. Of these "big data" collections, retrieval and processing of archives of scientific publications are particularly challenging, as they differ from conventional texts due to vastly different usages of words and phrases within individual disciplines. In this work, inspired by the way operations of information storage and retrieval in human memory are represented, we build an associative model of words from scientific corpora. The idea is to assume that associated or similar words often appear together in the same texts. To measure similarity between words, we use a contingency table, which records the appearances of words in publications. We use the table to compute a similarity score between -1 and 1, with 1 denoting that the words always appear together and -1 denoting that the words never appear together. The final goal is to optimize our method such that it can determine the similarity score between two pieces of scientific publications without human input. This technique differs from a commonly used method, called latent semantic analysis, in its flexibility, as factors such as multiplicities of words in texts and their proximity can be easily taken into account. Furthermore, unlike semantic analysis which averages over multiple meanings of a word, this method has the ability to discover multiple meanings based on context. Further development of the technique requires testing different methods of calculating similarity scores, recognizing words with different meanings based on their contexts, as well as optimizing to improve performance.



Introduction

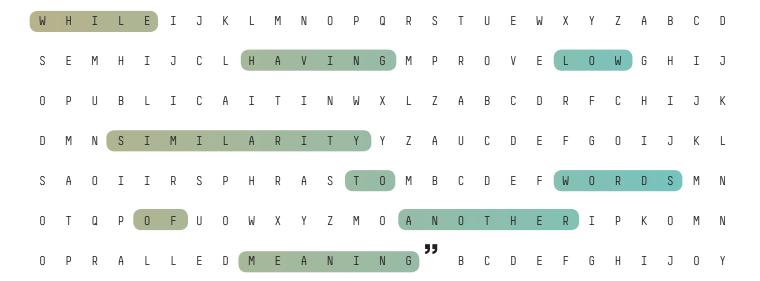
In the modern era of technology, lack of information is no longer a primary issue. On the contrary, data sets have become so large and complex that effective storage, retrieval, and analysis are difficult to implement. Collections of these large data sets have been coined "big data". Big data inundate users with so much information that it becomes hard to filter out desired results. Thus, we require more advanced methods of information retrieval, which refers to finding information relevant to specific queries in data sets.

One type of big data of interest, archives of scientific publications, utilizes particularly ineffective information retrieval. It is currently approached in such a way that the search results capture similarities among scientific papers neither intuitively nor satisfactorily. For instance, many search algorithms look exclusively for keywords. However, in cases where papers coin new words or if a word has different spellings or forms, these algorithms are ineffective. The Distributed Information Systems Group at Caltech, with whom I have been working, suggested an alternative approach to information retrieval: associative search, where the search system returns data units that are intuitively associated to the provided search terms. This approach was inspired by the way the brain recalls memories, and is hypothesized to be effective not only for scientific publications, but for other data as well.

Preparing and Trimming Abstracts

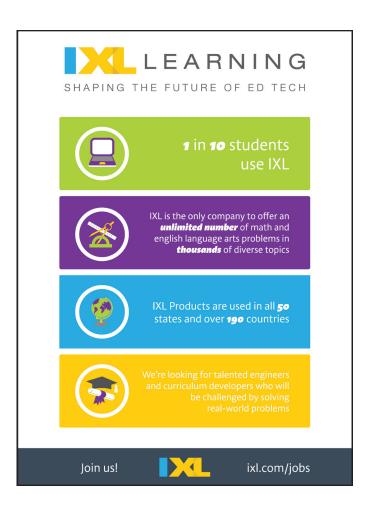
The main problem was to design an approach that would effectively group similar words in a way that could facilitate further development of searching for closely related documents. For instance, a pair of similar words would be "secret" and "wiretap", while "estimation" and "wire-tap" would be dissimilar. We extracted this information solely from the occurrences of words in the data, without human input. The goal was to boil the similarity of every pair of words down to a similarity score between -1 and 1. As an example, "secret" and "wire-tap" would have a high similarity score, while "estimation" and "wire-tap" would have a low similarity score. Related ongoing work in the lab included a project for developing algorithms that could solve remote association tests without direct human input but by using large human-generated networks of words. These remote association tests provide three common stimulus words, and the algorithms must solve the test by outputting a common fourth word.

The first step was to pick a corpus from which to study word similarities. We picked the Cornell University archive of scientific publications, arXiv, which contains a large amount of scientific papers. This archive contains more than 60,000 papers within the field of computer science alone.. We decided to study just the abstracts, as they would provide key terms in a relatively short amount of text. We downloaded the abstract meta data from the arXiv website and wrote the page sources to one text file (roughly 100 MB for 64,000 abstracts).



The next step was to trim each abstract in order to get rid of stop words, which, in the context of this paper, are words that do not provide scientific meaning. Examples of stop words include "the", "a", and "we". The purpose of this was to decrease the time it took to parse the data by decreasing the number of words we would need to consider. Another reason was to eliminate the effects of these words on similarity of documents. Consider two documents that do not contain similar scientific words but have similar stop words. Without removing these stop words, they would achieve high similarity scores when ideally, they should not. Next, with the trimmed text, we iterated through each word and recorded a list of unique words. At first, we received a total count of 140,000 unique words. With this list of words, we created a sparse matrix contingency table to record the existence of words in abstracts. These contingency tables are tables that record the appearances of words in abstracts in a sparse matrix in order to exploit the assumption that words only appear in a few papers. While columns represented abstracts, rows represented words. Each element in the matrix was either 1 or 0, 1 if the word is in the abstract and 0 if it is not. We achieved this step by running the data in Python, taking about six hours. With $\binom{140,000}{9}$ words, we would require a vast number of similarity scores (roughly 10 billion).

Looking through the list of words, we found that a majority of words that appear very few times were parts of equations written in LaTeX. To solve this issue, we simply removed any word that appeared in only one abstract. This cut our word count down to about 60,000, more than halving our original number.



However, this still left us with about two billion similarity scores to compute. We decided to switch to C++, opting to use a vector of maps over a sparse matrix library for simplicity.

Computing and Comparing Similarity Scores

In computing similarity scores, we used three methods: Cosine Similarity, Normalized Google Distance, and the Pearson product-moment correlation coefficient. In the following equations, f(x) denotes the number of abstracts containing word x, f(y) denotes the number of abstracts containing word y, and f(x, y) denotes the number of pages containing both x and y.

Cosine similarity is defined as

$$\frac{f(x,y)}{\sqrt{f(x)f(y)}} \tag{1}$$

It is the cosine between the vectorized word rows, hence the name. Cosine similarity scores are between 0 to 1, with 1 being most similar.

The Normalized Google Distance (Cilibrasi and Vitanyi, 2007) is defined as

$$\frac{\max\{\log f(x), \log f(y)\} - \log f(x,y)}{\log N - \min\{\log f(x), \log f(y)\}\}}$$

Its scores range from 0 to infinity, with 0 being most similar.

The Pearson product-moment correlation coefficient is defined as

$$\frac{f(x,y)}{N} - \mu(x)\mu(y) = \frac{\int_{N}^{\infty} -\mu(x)\mu(y)}{\sqrt{\mu(x) - \mu(x)^{2}}\sqrt{\mu(y) - \mu(y)^{2}}}$$
 (3)

where $\mu(x) = \frac{f(x)}{N}$. Its scores are normalized from -1 to 1, with 1 being most similar.

Initially, I computed similarity scores using cosine similarity, given by equation (1). [Figure 1] displays a table of similarity scores for six selected words. The diagonal contains all ones because it contains the similarity scores for a word and itself. The bottom triangle of the table is blanked out because the table is symmetric. Despite cosine similarity providing good

numbers for words that appear semi-frequently (between 5 to 20 percent of abstracts), they performed poorly for pairs of words in which at least one word appears very frequently (more than 20 percent of abstracts).

Examples of such words include "paper", "present", and "algorithm". These words had high similarity scores with most other words simply because they are generic words that appear very often, but were not filtered out as stop words. Furthermore, consider two words that appear independently and with probability in each document. Because their occurrences are independent, their similarity score should ideally be zero. However, the cosine similarity depends on in a monotonically increasing manner. As a result, we switched to equations (2) and (3), and decided to compare their relative performances as a side objective.

To do this, we calculated all similarity scores between one word and every other word using each equation, producing two lists of similarity scores. In order to determine the similarity between these two lists (and hence, the similarity between equations (2) and (3)), we used the Kendall tau rank correlation coefficient (equation (4)). Specifically, we used the -b version of Kendall's tau that accounts for ties, defined as

$$t = \frac{[P-Q]}{\sqrt{[P+Q+T][P+Q+U]}}$$
 (4)

where P is the number of concordant pairs, Q is the number of discordant pairs, T is the number of ties in the first list, and is the number of ties in the second list.

To test the similarity between Google similarity distance and the Pearson product-moment correlation coefficient, we randomly selected 1,000 words from our database. After running both equations on the 1,000 words, we computed the Kendall tau rank correlation coefficient for each pair of similarity score lists, resulting in a total of 2,000 lists.

At first, the calculations gave us unexpectedly low coefficients, never exceeding 0.4. We expected the numbers to be at least above 0.6. Revisiting the equations, we noticed that Google similarity distance gave every pair of words that never appear in the same abstract a score of infinity. On the other hand, the Pearson product-moment correlation coefficient had different degrees of negativity for pairs that never appear in the same abstract, depending on their frequencies. In other words,

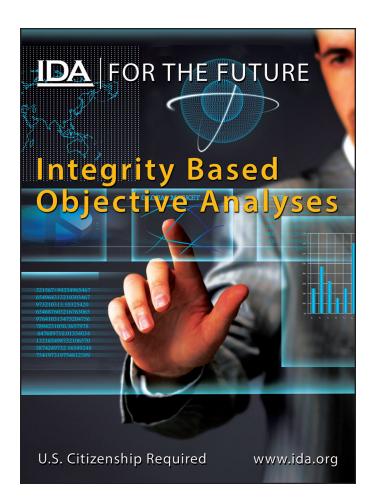
	secret	estimates	paradigm	minimize	compressed	wire-tap
secret	1	0.00309	0.00901	0.01001	0.00822	0.05976
estimates	-	1	0.01071	0.01814	0.02609	0.00592
paradigm	-	-	1	0.01431	0.02405	0.00574
minimize	-	-	-	1	0.01326	0.0
compressed	-	-	-	-	1	0.00629
wire-tap	-	-	-	-	-	1

Figure 1: A table of cosine similarity scores. The similarity score of "secret" and "wire-tap" is high signifying high correlation, while that of "minimize" and "wire-tap" is 0, signifying little similarity.

Pearson product-moment correlation is a two-sided measure that also measures dissimilarity, while the Google similarity distance is one-sided and assigns a single value for "dissimilar" words. To obtain a better understanding of the relationship between these similarity measures, we defined a modified one-sided Pearson product-moment correlation coefficient as

$$\max\{\frac{\frac{f(x,y)}{N}-\mu(x)\mu(y)}{\sqrt{\mu(x)-\mu(x)^2}\sqrt{\mu(y)-\mu(y)^2}},0\}$$

The result of this equation was a Pearson correlation coefficient that, like the normalized Google distance, also assigned a single value for dissimilar words. We then compared the Google similarity distance with the modified Pearson coefficient. The resulting calculations showed that the two equations produced numbers that ranked words very similarly. Over the 1,000 words, the mean Kendall tau rank correlation coefficient was 0.78606, with a standard deviation of 0.104907. [Figure 2] gives the results of this test, showing the distribution of Kendall tau coefficients. In fact, computing the coefficient for the 100 most similar words yielded scores no lower than 0.87. It is only when the lower ranked pairs begin having very low similarity scores that the equations deviate in ranking. As similarity between documents is more affected by highly similar pairs of words, we determined that the relative ranking of lower words are not particularly important, so long as they are low. In other words, similar words are successfully ranked highly for both equations, and dissimilar words are ranked lowly.



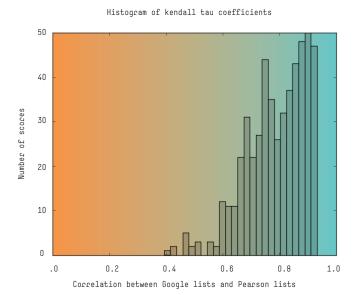


Figure 2: Histogram of Kendall Tau Coefficients.

Essentially, these computations showed us that modified Pearson coefficient and Google similarity distance produce extremely close similarity rankings. This tells us that before modification, the Pearson coefficient actually provides more information, since it tells us degrees of how dissimilar pairs of words are, while the Google similarity distance does not. As a result, we opted to use only the Pearson product-moment correlation coefficient in computing the similarity scores.

Remote Association Tests

To test the accuracy of using only the abstracts as our source of data, we decided to test our data using remote associates tests (RATs). These tests provide three related words, and the goal of the test is to provide a fourth word which best connects the given words. Yue Li, a member of the lab, had previously developed a dense graph created by user input and a solver algorithm to perform RATs on common words. Borrowing his program, we ran RATs on a few words we selected. For instance, giving the RAT solver "homomorphic", "key", and "encryption", we received the answer "security", which we had guessed. In [figuce 3], we arbitrarily choose two words with rounded similarity scores as an example. The RAT picks "security" as a solution despite the "homomorphic"-"isomorphic" pair having the highest similarity score, because "security" is more closely related to all three inputs. Unfortunately, there is only manual checking for the tests, limiting the number of possible tests, but the solver provided reasonable answers for the tests we did perform.

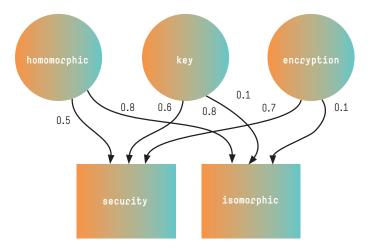


Figure 3: Example RAT. "security" has a combined similarity score of 1.8 with the three inputs, while "isomorphic" only has a score of 1. Thus, we choose "security" despite the "homomorphic"-"isomorphic" score being the highest in our graph.

Abstract Similarities

After settling on using the Pearson correlation coefficient as our similarity score and testing the reliability of abstracts, we next decided to test how effective it was at comparing the similarity between two abstracts. To achieve this goal, we used the following equation.

$$S(A_{1}, A_{2}) = \sum_{\forall i \in A_{1}, j \in A_{2}} \frac{s(i, j)}{|A_{1}| |A_{2}|}$$
 (5)

where A_1 is the set of unique words in the first abstract, A_2 the set of unique words for the second, and s is the similarity score between words i and j. In essence, we created a bipartite graph from the two abstracts, and edges are similarity scores. We then averaged these scores to obtain a final score for the similarity between the two abstracts. We decided to give the similarity score a lower bound of 0.02, as testing many different papers that cited each other resulted in this value being the minimum. By checking manually, we observed high similarity in pairs that yielded similarity scores higher than 0.02.

Unfortunately, many papers received similarity scores that broke the 0.02 threshold with short abstracts that contained very commonly used words ("paper", "present", "algorithm", etc.). Our attempt to solve this problem by switching from equation (1) to equation (3) did not work, and thus it was not completely fixed. As a result, we decided to go through the list of unique words and manually trim out words that we believed to have no

"The idea is that if a word has at least two different meanings, the words associated with one meaning will have high similarity with respect to each other, while having low similarity to words of another meaning."

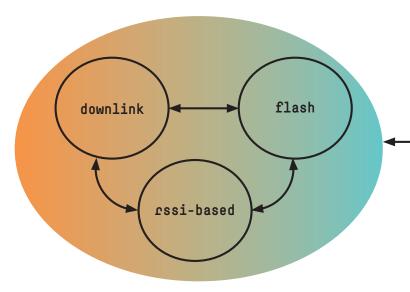
specific scientific meaning. After this modification, the previous problem no longer had a large impact. For instance, for a particular paper, the topic of which is pebble games and sparse graphs, all abstracts with similarity score 0.02 and above were either cited by that paper or authored by the same authors. Note that we only used citation or authorship information for testing purposes; our actual method neither uses nor requires it. As a result, even if citation and authorship information are missing, our method is capable of discovering similarity between two abstracts.

Multiple Word Meanings

The next step of the project was to develop a method of determining whether a word had multiple scientific meanings. The idea is that if a word has at least two different meanings, the words associated with one meaning will have high similarity with respect to each other, while having low similarity to words of another meaning. As an example, consider the word "foot", with one meaning related to the body part and the other to the unit of measurement. In the some contexts, "foot" is similar to "hand" and "leg", while in others, it is closely related to "inch" and "meter". Thus, among the words that are closely related to "foot", there are different degrees of similarity: "inch" and "meter" are similar but "inch" and "hand" are not.

To exploit this property in order to find the different contexts of words with multiple meanings, we took a word, found all of its similarity scores with all other words, and kept the words





with scores above 0.05. With these words, we created a complete graph, with the edge weights being the similarity scores between vertices, which are the words. To partition the graph into groups of words that are related to the different meanings and contexts of the chosen word, we found a min-cut, which is the line dividing the vertices that goes through the smallest sum of edge weights. This should provide us with the proper cut between two groups. We repeatedly pruned vertices that had edges to more than 80% the number of total vertices and vertices that had only one neighbor. At first, we attempted to use Karger's algorithm, but soon decided to use another algorithm as described in "A Simple Min-Cut Algorithm" [Stoer and Wagner, 1997], which provides a better time complexity. With this basic implementation, we selected several words that had different meanings. For instance, for "cell", which has meanings in both biology and electrical engineering, we received the following min-cut.

First group of vertices:

cellular dendritic dca stations inter-cell multi-cell downlink multicell station bs uplink per-cell base immune-inspired eicic hetnets macrocell flash femto word-line rssi-based powerxcell antigen bss immune handovers cell's ofdma macro cgi k-cell two-cell mobile

Second group of vertices:

protoplasmic polycephalum attractants nutrients plasmodium imitated unaided physarum

However, we expected *dendritic, immune-inspired, immune, antigen* and *dca* to be in the second vertex, since they are all biology topics. Furthermore, with some variations of pruning thresholds, the second vertex would only contain cell's. We believed that the first problem could be solved by performing multiple min-cuts, while the second could only be solved by getting rid of variations of the word in question.

After, we successfully received a third group of vertices: dendritic immune-inspired immune antigen dca
Similar situations were found and solved for other words with multiple meanings, such as "bias", "code", and "error".

Conclusion

The results we obtained from each step of the process have been highly satisfactory. We believe that in order to increase the accuracy of our technique, we would have to perform our previous methods on the entire papers, rather than just the abstracts. This would take significantly more time, but would provide even better results. If successful, we would be able to show a method that provides features that latent semantic analysis would not provide, such as the min-cut of multiple meanings. In addition, we would have better performance, since latent semantic analysis has been shown to be ineffective for massive web data sets due to its singular value decomposition method (Cilibrasi and Vitanyi, 2007).

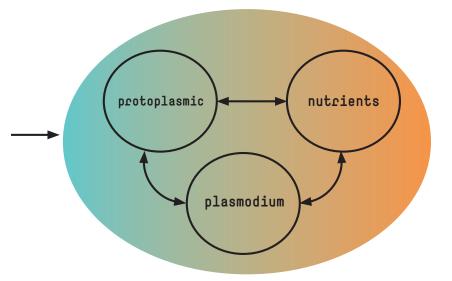


Figure 4: In this example, all six words are in the list of those most related to "cell". Though not every edge is shown, it is a complete graph. The edge linking the two three-word-bubbles consists of the 9 edges (each node from each bubble to each node of the other) through which our min-cut goes. Those 9 edges have a combined similarity scores no greater than any other possible combination of 9 edges. If the cut's weight exceeds a certain threshold, then we know we have at least two meanings for a particular word.

Further work on the project would require us to parse entire papers instead of abstracts in order to increase accuracy of our similarity scores.

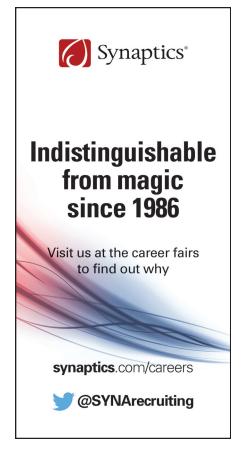
Acknowledgements:

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Bibliography:

Cilibrasi, Rudi, and Paul M.B. Vitanyi. "The Google Similarity Distance." IEEETransactions on Knowledge and Data Engineering: 370-383. Print.

Stoer, M. and Wagner, F. (1997). A Simple Min-Cut Algorithm. Journal of the ACM}, 44:585--591. Leskovec, Jure, Anand Rajaraman, and Jeffrey D. Ullman. Mining of assive datasets. New York, N.Y.: Cambridge University Press, 2012. Print.

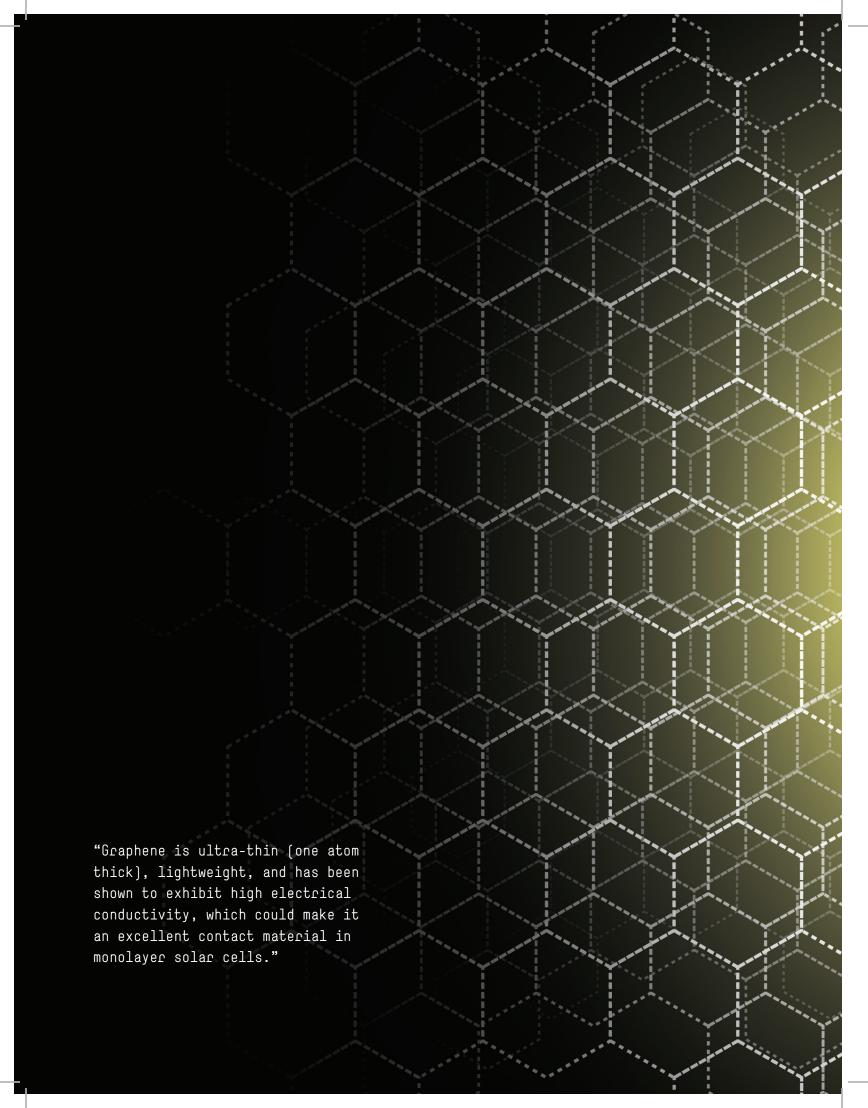




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Novel Monolayer Materials and Geometries for Ultra-lightweight High-efficiency Solar Cells and Plasmonics: MoS2 and Graphene



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ABSTRACT:

Monolayer materials have remarkable electrical and optical properties that differ tremendously from their bulk counterparts. Some monolayer materials that are now being heavily researched are graphene and MoS2 because of their potential in applications such as monolayer solar cells and plasmonics. Due to its ultra-thin characteristic, graphene can be used to fabricate effective plasmonic devices which can then be analyzed using a technique called angle-resolved cathodoluminescence (CL) nanoscopy. Angle-resolved CL nanoscopy relies on focused electron beams on samples that scatter cathode rays at mid infrared to visible wavelength ranges. A detector collects these cathode rays and are able to determine properties such as optical modes and plasmon resonant frequencies of the devices. These insights would better explain the fundamental physics behind how plasmons behave in the devices which can lead to more exciting applications. Graphene has also been shown to exhibit high electrical conductivity, which could make it an excellent contact material in monolayer solar cells. Another material that is ultra-thin and lightweight is ${\sf MoS}_2$ which is different from graphene in that it is a direct bandgap semiconductor whereas graphene has no bandgap and is thus considered a semimetal. MoS_2 has been shown to absorb up to 10% incident sunlight in a thickness of less than 1 nm, which is an order of magnitude greater than current materials used for solar cells, such as GaAs (gallium arsenide) and Si. 1 The motivation behind using MoS₂ is that it acts as a good monolayer semiconductor that has low series resistances, large voltage capacities, and near-optimal I-V (current to voltage) curves. Coupled with metal-like materials like graphene, MoS_2 can be used to create optimal monolayer solar cells, such as Schottky junction solar cells. However, efficiencies of monolayer solar cells often suffer from the losses that take place during light absorption. Implementing a light trapping technique will help to improve the light absorption of the MoS2 which will increase the overall effi-

ciency of the solar cell.

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Graphene, with its unique and fascinating characteristics, is one of the most versatile materials currently researched today. A simple two-dimensional lattice of carbon atoms, graphene has remarkable electrical, mechanical, and optical properties. Graphene has an electrical mobility that can be as high as $200000 \text{ cm}^2 - \text{V}^{-1} - \text{s}^{-1}$, a 2.3% light absorption per nanometer which is orders of magnitude more light absorption than bulk materials like silicon and gallium arsenide, and a tensile strength of 130 gigapascals (10^9) at the small weight of 0.77 milligrams per square meter (about 0.001% of the weight of 1 square meter of paper) compared to steel's tensile strength of 400 megapascals. Because of these unique properties, graphene can be used for structural materials, biomedical applications, an emerging field known as plasmonics, and solar cells.

KEYWORDS: Schottky junction, graphene, plasmonics, solar cells, light absorption, direct bangap semiconductors, semimetals, angle-resolved cathodoluminescence nanoscopy

As an application for monolayer solar cells in particular, graphene is ultra-thin (one atom thick), lightweight, and has been shown to exhibit high electrical conductivity, which could make it an excellent contact material in monolayer solar cells. Graphene by itself cannot be used to create a solar cell as it is a semimetal and has no bandgap. A bandgap is the difference in energy between the highest energy state in a valence band and the lowest energy state in a conduction band and signifies the amount of energy an electron can release after excitation by light. The two different types of bandgaps are indirect and direct. Indirect bandgaps involve changes in both energy and momentum and are not ideal for solar cells because of the losses in energy efficiencies due to momentum changes. Direct bandgaps are ideal because they do not involve changes in momentum which results in more available usable energy from excited electrons. A group of materials that is ultra-thin, lightweight, and are direct bandgap semiconductors is the transition metal dichalcogenides (TMDs). One type of TMDs, MoS2, has been shown to absorb up to 10% incident sunlight in a thickness of less than 1 nm, which is an order of magnitude greater than cur-

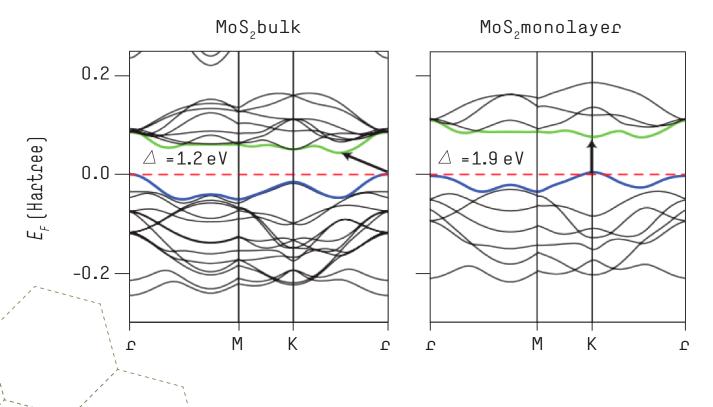


Figure 1: The bandgap structures of bulk (left) and monolayer MoS $_2$ (right), which are calculated from first-principles density functional theory. The y-axis is energy and the x-axis is momentum. Bulk MoS $_2$ has an indirect bandgap of 1.2 eV while monolayer MoS $_2$ has a direct bandgap of 1.9 eV. $_4$

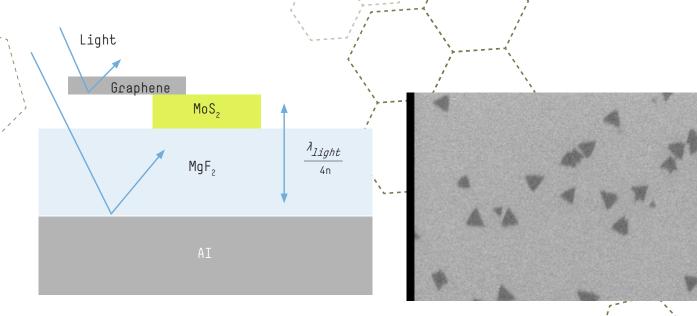


Figure 2: Preliminary layout of solar cell with MoS2 and graphene Figure 3: The black triangles are the MoS2 grown on SiO2 substrates. used in this light trapping technique.

rent materials used for solar cells, such as GaAs and Si. 1 The motivation behind using monolayer MoS2 is that it acts as a good semiconductor that has low series resistances, large voltage capacities, and a low direct bandgap energy of 1.9 eV as seen in Figure 1.4

Coupled to other materials with metallic properties like graphene, semiconducting MoS_2 can be used to create optimal monolayer solar cells, such as Schottky junction solar cells. A Schottky junction is an interface between a semiconductor and a metal and previous research has shown that effective solar cells can be fabricated from graphene and silicon.⁵ In fact, new research shows that Schottky junction solar cells have a power density 4 to 5 times greater in magnitude than traditional silicon solar cells. Although the concept of monolayer solar cells is great due to their lightweight properties and high efficiencies, an issue that arises is the overall light absorption. Monolayer solar cells are significantly thinner than typical solar cells and thinner films usually absorb less light which results in low solar cell efficiencies of 0.1 – 1.0%. A technique that can solve this issue is known as light-trapping. The light-trapping technique that will be implemented in the experiment can be seen in Figure 2. This involves using destructive interference of incident light that is reflected by an aluminum layer and transmitted through an MgF₂ layer that has a thickness of one-fourth the wavelength of the incident light divided by the index of refraction of MgF₂.



The destructive interference will allow all the light to be concentrated on the ${\sf MoS}_2$ which will improve the light absorption of the monolayer material.

The method used to synthesize monolayer MoS_2 on Si/SiO_2 is chemical vapor deposition (CVD). The S and Mo sources are from elemental sulfur powder and MoO_3 powder, which are weighed into two alumina crucibles. The alumina crucibles are inserted into a quartz tube at different positions in a furnace. One zone in the furnace is used and is heated to between 600° C and 700° C for 43 minutes. The Mo source is placed directly into the heated zone with the Si/SiO_2 substrate on top of it, downstream of the S source and N_2 flow. Ultra high purity nitrogen gas is used to purge the tube at 5.0 SCFH (standard cubic feet per hour) and then the flow is decreased during the annealing process. A scanning electron microscope (SEM) image of the grown MoS_2 is shown in Figure 3.

To prepare MgF₂ on AI, electron beam deposition can be used. Electron beam deposition is a technique that uses electrons to bombard materials that turn into gaseous phases and condense on a substrate to form the desired depositions. Because MgF₉ and AI are commercially accessible materials, electron beam deposition can be used to deposit Al on a silicon wafer and then deposit MgF₂ on the Al layer. MoS₂ will be deposited using CVD and then graphene will be transferred onto the MoS2 once grown on copper using CVD (Figure 2). Graphene is grown on 99.999% pure copper where the first step of growth is H₂ being purged at 50 SCCM (standard cubic centimeters per minute) in a tube from 20°C to 800°C for 45 minutes. After 10 minutes of waiting, a 30 minute ramp from 800°C to 1000°C is performed before waiting another 255 minutes. CH₄ at 0.5 SCCM is added for 50 minutes before the furnace temperature is ramped down from 1000°C to 20°C for 50 minutes at 1 SCCM CH4 and 50 SCCM H2. Graphene is etched off copper using iron chloride, and then transferred onto the \mbox{MoS}_2 which will have already been grown on the ${\rm MgF}_2$ and Al layers using CVD.

To test the quality of the ${\rm MoS}_2$ and graphene grown, equipment such as Raman spectrometers and power meters are used. The power meter collects reflection and transmission measurements of the samples as a function of wavelength from a laser. Absorption can then be calculated by subtracting the sum of reflection and transmission from 100% [Figure 4].

High-quality ${\rm MoS}_2$ will have specific absorption properties which will be used to understand the potential of the material in photovoltaic devices. The two features in the 600 to 700 nm wavelength range represent at what wavelengths monolayer ${\rm MoS}_2$ absorbs the most. The 10% maximum absorption that is seen for this monolayer ${\rm MoS}_2$ sample agrees with previous work done by Bernardi which suggests that this is a high-quality sample.

Raman spectroscopy relies on inelastic scattering of monochromatic light from a laser. The laser light interacts with the sample causing various excitations such as molecular vibrations or phonons. These excitations can be recorded as peaks that vary in energy and amplitude. The quality of grown material can then be determined by analyzing the Raman peaks (Figure 5). The Raman profiles indicate whether the ${\rm MoS}_2$ is monolayer or multilayer based on the ratio of the counts of the silicon Raman peaks to the ${\rm MoS}_2$ peaks.

The higher the ratio of the silicon peak counts to MoS_2 peak counts, the more multilayer the MoS_2 becomes. In addition, MoS_2 Raman peaks that are closer together represent

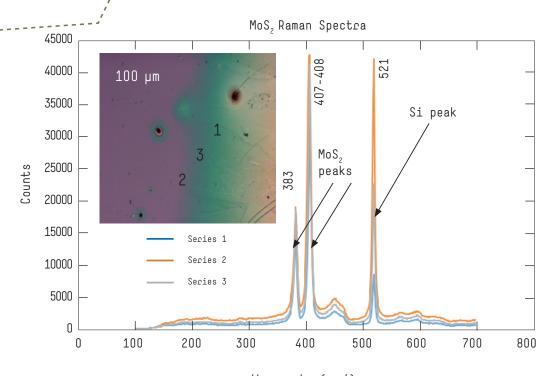


more monolayer MoS_2 regions. For the series 2 Raman profile, the MoS_2 peak is at 407 rather than 408 cm⁻¹. Thus, based on the Raman spectra collected, position 2 on the optical image seen represents monolayer MoS_2 [Figure-5].

Once the entire monolayer solar cell has been fabricated, the 4-point probe can be used to generate an I-V curve to show how much electrical resistance the solar cell has. An I-V curve maps the current through the material as a function of applied voltage. According to Ohm's law, the relationship between current and voltage is expected to be linear with slope 1/R where R is the resistance of the material. Low resistances are ideal because they allow more current to flow through solar cells. Solar simulators can calculate the overall efficiency of the solar cell by flashing light at the same frequency as sunlight, and finding the output current as a function of voltage.

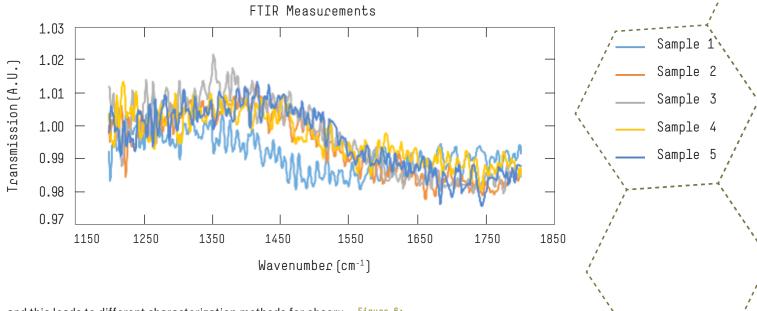
Another noteworthy application of graphene is plasmonics. Plasmonics is the study of wave-like oscillations of electrons in materials like metals which has applications to on-chip optical

signal routing and to understanding the physics behind lightmatter interactions. 6 More specifically, surface plasmon polaritons (SPPs) are optical modes of an evanescent wave in a dielectric coupled to an oscillating wave of charge on the surface of a conductor.⁶ The properties of these modes are large wavelength reductions relative to free space and optical dispersion relations that can be engineered via metal/dielectric nanoarchitectural design. The problems with using traditional metals as plasmonic materials is that they have low carrier mobilities, surface roughness, and grain microstructure and impurities which lead to losses in electron oscillations.8 In addition, the large electronic density of states in metals restricts the turing of the plasmon energy via electrostatic fields. 6 Because it has been shown that SPPs excited on metal films that are embedded in dielectrics have smaller mode volumes as the metal layer becomes thinner, a one atom thick material like graphene would have its SPPs display the smallest mode volumes, which result in very strong light-matter interactions. 9-15 The study of graphene as a plasmonic material is still relatively new



Wavenumber(cm⁻¹)

Figure 5: The Raman profile for MoS2 grown on Si. The right most peak located at wavenumber 521 represents the presence of Si and the two peaks at wavenumbers 383 and 407-408 represent the presence of MoS2. Series 1, 2, and 3 represent the different positions of MoS2 profiled using Raman spectroscopy, which can be seen on the optical image. The light blue area represents multi- and monolayer MoS2 grown. Series 2 represents the area of MoS2 that is most similar to monolayer.

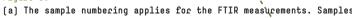


and this leads to different characterization methods for observing and analyzing its physics such as FTIR (Fourier transform 2-5 have dips at 1700 cm-1 whereas sample 1 has a dip at 1500 cm-1 infrared) transmission measurements and SEM imaging.

In order to fabricate the devices for the plasmonics experiment, high quality graphene is essential. Graphene is grown similarly as it was for the solar cell experiment. The graphene is then transferred onto silicon wafers with 285 nm SiO₂. Nanoresonator arrays were then patterned in the graphene using electron beam lithography on 90-300 nm thick 950 PMMA (polymethyl methacrylate) and then etched using oxygen plasma at 20 milliTorr and 80 Watts for 10 seconds. The exposed PMMA was developed in 3:1 isopropanol:methyl isobutyl ketone (MIBK) for 45 seconds. Source and drain contacts in the form of gold were deposited on the graphene using thermal evaporation in order to control the carrier density of the device. Once the devices have been fabricated, they were put under focused electron beams from a scanning electron microscope (SEM) for various amounts of time. SEM images of the graphene devices with different exposure times were taken in order to qualitatively determine the effect of the focused electron beam. Visible effects on the graphene devices were only seen at exposure

For a more quantitative measurement, FTIR (Fourier transform infrared) transmission spectroscopy is used in order to determine the quality of the devices that are exposed to varying levels of focused electron beams (Figure 6a). From Figure 6a, it can be seen that one sample one has a dip at 1500 cm⁻¹ and samples 2-5 have dips at 1700 cm⁻¹. Sample one's undoped graphene has a dip at 1500 cm⁻¹ which is indicative of its plasmon resonance.

times that were more than 10 minutes (Figure 6b).





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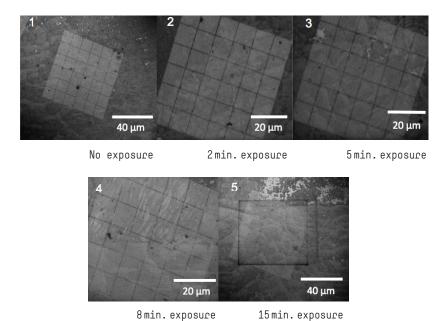


Figure 6: (b) SEM images taken with a focused electron beam at 5 kV and $0.4\,$ nA at different times of exposure.

However, graphene devices exposed to focused electrons have dips at 1700 cm⁻¹ which suggests that the devices that are exposed are doped with electrons, thus giving them an increase in energy. This implies that the devices are not badly damaged or destroyed when angle-resolved CL nanoscopy is performed since it relies on focused electron beams that hit the sample and cathode rays that are scattered off the sample and collected within the near infrared and visible wavelength ranges. Angle-resolved CL nanoscopy can be used to detect the plasmon resonant frequency as a function of position and wavelength. This functionality allows for the detection of resonant modes of electrons analogous to a particle-in-a-box resonances. Using angle-resolved CL nanoscopy to analyze the graphene devices at the subwavelength range and with angleresolved detection capabilities will shed more light on the fundamental physics behind plasmonics.

Overall, monolayer materials such as graphene and ${\rm MoS}_2$ have remarkable electronic and optical properties that can be used for various applications such as photovoltaics and plasmonics. As a direct bandgap semiconductor, monolayer ${\rm MoS}_2$ can be used to fabricate monolayer solar cells that have a lot of potential despite having low levels of absorption. Graphene, which is one atom thick, has no bandgap and thus can be substituted as a metal which will enhance the efficiencies of solar cells and help to discover the underlying physics behind plasmonics.

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References

- 1 Bernardi, M., et al. Nano Letters 2013, 13, 3664-3670.
- 2 Chen, J., Jang, C., Xiao, S., Ishigami, M., Fuhrer, M. S. Nature Nanotechnology 2008, 3, 206-209.
- 3 Geim, A. K., Novoselov, K. S. Nature Materials 2007, 6, 183-191.
- 4 Wang, Q. H., et al. Nat Nano 2012, 7, 699-712.
- 5 Li, X., et al. Advanced Materials 2010, 22, 2743-2748.
- 6 Brar, V. W., et al. Nano Letters 2013, 13, 2541-2547.
- 7 Raether, H. Springer-Verlag 1988, p x.
- 8 Nagpal, P., Lindquist, N. C., Oh, S.-H., Norris, D. J. Science 2009, 325, 594-597.
- 9 Berini, P. Opt. Lett. 1999, 24, 1011-1013.
- 10 Dionne, J. A., Sweatlock, L. A., Atwater, H. A., Polman, A. Phys. Rev. B 2005, 72, 075405.
- 11 Miyazaki, H.T., Kurokawa, Y. Phys. Rev. Lett. 2006, 96, 097401.
- 12 Kliewer, K. L., Fuchs, R. Phys. Rev. 1967, 153, 498-512.
- 13 Economou, E. N. Phys. Rev. 1969, 182, 539.
- 14 Sarid, D. Phys. Rev. Lett. 1981, 47, 1927-1930.
- 15 Burke, J. J., Stegeman, G. I., Tamir, T. Phys. Rev. B 1986, 33, 5186-5201.

