REU PHYSICS & ASTRONOMY RESEARCH SYMPOSIUM

Summer 2011

STONY
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STATE UNIVERSITY OF NEW YORK

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RESEARCH EXPERIENCES FOR UNDERGRADUATES (REU)

Physics & Astronomy Research Symposium

2 August 2011

OPENING STATEMENTS AND ACKNOWLEDGEMENTS—

9:25 Dr. Erlend Graf, REU Physics Director

UNDERGRADUATE PRESENTATIONS

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9:45	Benjamin Chonigman
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CLOSING REMARKS—Dr. Erlend Graf

***All abstracts will be posted on the REU PHYSICS Website:
http://www.stonybrook.edu/ureca/physicsreu

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INTRODUCTION

Stony Brook University is proud to host the Research Experiences for Undergraduates (REU) Program in Physics & Astronomy. Sponsored by the National Science Foundation (NSF), this program gives undergraduate students an intensive hands-on research experience and involves them in all phases of the research process. This year, ten summer researchers from colleges and universities throughout the country were selected from a select pool of approximately four hundred applicants. In carrying out their projects, REU participants worked alongside Stony Brook's faculty, post-docs, graduate students and other undergraduates. The summer activities culminated in a presentation of the students' work in a research symposium and in a written report.

As you read this collection of their abstracts, you will see evidence of their hard work, keen insight and enthusiasm, and be impressed at what they have accomplished in approximately eight weeks. I have no doubt that these individuals will continue on with successful academic and research careers.

—Erlend Graf, Director, REU Physics & Astronomy program, Stony Brook University

Michele Silverstein
Cornell University

Hints of planet formation in nearby young moving groups

Michele Silverstein, *Cornell University*; Ana-Maria Constantin, *International Computer High School of Bucharest (Simons Program)* ; MICHAL SIMON, *Department of Physics & Astronomy, Stony Brook University*

The main goal in this project is to detect debris disks using the WISE database in several nearby young moving groups. The WISE, Wide-Field Infrared Survey Explorer, database is a survey that covers the entire sky in the 3.4, 4.6, 12 and 22 micron bands. A debris disk surrounds a star and is composed of dust and planetesimals, the remnants of planet formation. The parallel to this in our own solar system is the Kuiper Belt. A moving group is a cluster of stars of similar properties, such as age and chemical composition, traveling together. We studied nearby young moving groups, with ages of 5-150 million years, very young compared to our 4.6 billion year old Sun. Stars with debris disks may have planets and be able to teach us more about planet formation. For this reason, the detection of debris disks is a worthy goal in seeking out exoplanets. Detection of debris disks around stars in a moving group is also valuable, since stars in the moving groups are very nearby and young. Planets around young stars are more luminous and therefore easier to detect. In short, debris disks around a star in a nearby young moving group would increase the chance of finding a planet around the star. Our first step in this project was to establish whether or not the WISE database could be used to detect debris disks. It turns out this is possible using color-color diagrams, but not for all debris disks; some debris disks go undetected. Our results are also unavoidably incomplete due to the release of WISE data for only 60% of the sky. Once a viable method of detection was established, we used this method to search for debris disks in five of the nearby moving groups: AB Doradus, the Tucana-Horologium Association, Beta Pictoris, Epsilon/Eta Chameleon and TW Hydrae. We also investigated a section of the color-color diagrams where stars in the moving groups overlap the region ordinary stars. Our results are we (1) confirmed the existence of previously known debris disks and (2) identified new debris disks, where (3) the youngest moving groups have the most debris disks detected.

Benjamin Chonigman
Stony Brook University

Space charge limitations on current for a Cs negative-ion sputter source

Benjamin Chonigman, Akshat Puri, *Stony Brook University*; Jason Chaves, *Stanford University*; Camilla Dagum, *Cornell University*; Richard Lefferts, Andrzej Lipski, THOMAS K. HEMMICK, *Center for Accelerator Science and Education (CASE), Department of Physics & Astronomy, Stony Brook University*

Accelerator Mass Spectrometry (AMS) is a technique to measure the presence of different isotopes of the atoms in a sample by ionizing the atoms in the sample and then accelerating them to high kinetic energies. In order to equip the tandem Van de Graaff Accelerator used in the Center for Accelerator Science and Education (CASE) at Stony Brook University to be able to do AMS, last summer a new Cs negative-ion sputter source was designed as to increase the negative-ion currents formed. The new ion source design features a molybdenum spherical ionizer to ionize the neutral cesium vapor, a stainless steel "shroud" used to focus the Cs beam onto the sample as well as a Cs vapor vent and a stainless steel "immersion lens" to focus the negative-ion beam sputtering off the sample.

To confirm that the new ion source was producing the Cs currents of approximately 1 mA needed to get the necessary negative-ion currents we assembled the new ion source in a test stand. Tests were conducted without the immersion lens and using an aluminum collector plate, placed approximately 10cm away from the shroud, as the cathode to collect and measure the Cs current. After baking contaminants off of surfaces and pumping the system down to high vacuum (10^{-5} to 10^{-6} torr) we found that even with a -15kV difference between the ionizer and the collector plate we were only able to get Cs currents on the order of 10 μA.

We realized that the reason the Cs currents were so far off from the expected currents of ~1mA was that as Cs atoms are ionized and accelerated from the ionizer to the collector plate the space between the ionizer and the plate fills up with a cloud of Cs+ ions known as space charge. Almost instantly this space charge builds up to the point that all the electric field lines leaving the cathode are terminated in the space charge and never reach the ionizer's surface. This means that as more Cs+ ions leave the ionizer they are repelled by the space charge and are sent straight back to the ionizer, effectively creating a limit on the amount of Cs current. This limit is dependent on the geometry of the cathode and ionizer as well as the mass and charge of the ions that make up the space charge. This relationship is quantitatively described for a parallel plate geometry by the Child-Langmuir Law $J = \frac{4\epsilon_0}{9}\sqrt{\frac{2q}{m}}\frac{V^{\frac{3}{2}}}{d^2}$; where J is the current per area of the collector plate, V is the voltage between the plates, d is the distance between the plates, and q and m are the charge and mass of the Cs ions.

As applied to our set-up, the Child-Langmuir Law states that the Cs current is inversely proportional to the distance from the ionizer to the cathode squared. Now understanding the importance of the distance we placed the collector plate in a more realistic geometry, about 4 cm away from the ionizer. However we still found that we were only able to get a max Cs current of ~0.2mA with the highest voltage available before the onset of sparking (~2kV).

Electric field calculations including the effects of space charge as done in SIMION 8.0.7 led us to decrease the height of the shroud by 0.320" while moving the ionizer that same distance closer to the sample. More testing will be required to see whether these modifications were sufficient to get the 1mA current needed.

This work was supported by a grant from the National Science Foundation (Phy-0851594).

Camilla Dagum
Cornell University

Measuring Cesium current from an ionizer

Camilla Dagum, *Cornell University*; Jason Chaves, *Stanford University*; Benjamin Chonigman, Akshat Puri, *Stony Brook University*; Richard Lefferts, Andrzej Lipski, THOMAS K. HEMMICK, *Center for Accelerator Science and Education (CASE), Department of Physics & Astronomy, Stony Brook University*

Accelerator Mass Spectrometry (AMS) is an exciting and relatively new technique for isotopic analysis. Our aim is to transform Stony Brook's tandem Van de Graaff accelerator, formerly used for nuclear physics research, into an AMS facility that can detect various radioisotopes in small samples (less than 1mg) and in short periods of time. AMS is also much more accurate than traditional low-level counting methods of radioisotopes, for it allows for complete rejection of molecular background; i.e., detection of a mass-14 substance could only be a carbon-14 or nitrogen atom.

The tandem accelerator requires negative source ions, created by a process known as "sputtering." A 5keV beam of cesium ions (Cs^{1+}) is focused on the sample, which will then sputter out positive and negative ions, as well as neutrals. An electrode sits below the ionizer at a positive potential to extract the negative ions. Through the optics of the system, the negatives are subsequently accelerated to a thin foil at a large positive voltage (~5 MV), where they are stripped of electrons so as to become positively charged, and are accelerated again to the detector.

We spent this summer coming to a full understanding of the first step in the AMS process: creating the cesium current. Cesium vapour is fed into the vacuum chamber onto a hot molybdenum ionizer, and a plate or rod with negative voltage (~-3kV) collects the current. Last summer a prior generation of students designed the ion source in principle. We took these plans and tested them to discover that there are far more limitations involved in this process than we had anticipated. Space charge, conductance of the vacuum, and containment of cesium in the area of the ionizer complicated our evaluations. After individually modifying and testing essentially every aspect of the ion source set up, however, we have concluded how to get the most cesium current and confidently look forward to completing the transition to an AMS facility.

This work was supported by a grant from the National Science Foundation (PHY-0851594).

Jason Chaves
Stanford University

Assembly and testing of a Cesium ion source for accelerator mass spectrometry

Jason Chaves, *Stanford University*; Camilla Dagum, *Cornell University*; Benjamin Chonigman, Akshat Puri, *Stony Brook University*; Richard Lefferts, Andrzej Lipski, THOMAS K. HEMMICK, *Center for Accelerator Science and Education (CASE), Department of Physics & Astronomy, Stony Brook University*

The first purpose of this work was to assemble the Cesium ion source on a preliminary testing stand. The parts for the ion source were based off the initial source that ran in Purdue University's PRIME Lab AMS facility. The ion source was assembled and attached to a metal stand. A turbo-molecular pump, backed by a roughing pump, was attached to one side of the ion source. The other side was fitted with a high vacuum ionization gauge and a current collecting cathode. Once it was shown that our ion source was leak-free, through the use of a portable Helium leak detector, and able to reach a high vacuum pressure of 10^{-7} torr, the purpose then moved on to test running the source, with the goal of acquiring an understanding of how external variables affected the Cs current and how to reach a maximum in this current.

In test running the ion source, we came to understand the importance of space charge in our system, which was greatly shifting the ion source behavior from what was initially expected and significantly limiting our Cs beam current. In over-simplified theory, the positive Cs ions are accelerated towards the sample, which is held at a high negative voltage, and so there would be no problem in having each ion contribute to positive beam current. In reality however, the positive potential from Cs ions in the positive beam repels the ions and prevents all of the ions from immediately becoming part of the beam current, effectively putting an upper limit on the beam current. We found that Child's Law is a theoretical formula that defines the upper limit for current between two capacitor-plate-like electrodes, where the upper limit has a functional form of constant x $V^{3/2} / d^2$, or $E^{3/2} / d^{1/2}$.

In order to predict how space charge limited our current and changed our beam optics, we used SIMION 8.0, which is a 3D electric field and ion trajectory modeling program. Adjustments had to be made to the existing SIMION model of the ion source, particularly scaling the model to real-life dimensions and writing a Python routine to create a new ion definition file to realistically model how ions would form off the spherical ionizer. The ions trajectories were simulated with space charge effects included and it became evident that space charge would indeed move our positive beam's focus to a point farther from the ionizer than originally designed. SIMION also allowed us to test several different alterations to the original ion source design to see how they affected the beam optics and electric field at the ionizer. The goal is to get the positive beam to focus as well as possible without having to move the sample in the design too much, while also maximizing the electric field at the ionizer since that is roughly what sets the upper limit on the beam current. We decided to decrease the height of the shroud and add a nozzle-shaped fitting to the immersion lens to help reach both of these goals.

We've ran the ion source under many different internal configurations and externally controlled voltages, ionizer temperatures, and Cs container temperatures in order to get a hands-on understanding of how the ion source responds to these changes. Thus far, we've been able to produce 200 μA of Cs current at will, but not continuously. Our target current is 1 mA, which is set by the amount of negative Carbon beam that we want to sputter off the sample, and we are confident that our new modifications to the shroud and immersion lens will allow us to reach that current in a stable fashion.

This work was supported by a grant from the National Science Foundation (NSF Grant Phy-0851594).

David Meltzer
Stony Brook University

Identifying the topological charge of optical vortices through diffraction

David Meltzer, *Stony Brook University*; MARTY COHEN, JOHN NOÉ, *Laser Teaching Center, Department of Physics & Astronomy, Stony Brook University*

This project studied the properties of optical vortices diffracted by hard apertures and how diffraction can be used to measure the topological charge of the vortex. Optical vortices are a type of transverse (spatial) laser mode that contains a phase singularity. Hermite-Gauss (HG) modes have rectangular symmetry while Laguerre-Gauss (LG) modes have cylindrical symmetry. It is well known [1] that cylindrical lenses can be used to convert HG laser modes to LG laser modes, and vice versa. The key feature of optical vortices, the singularity at the center of the beam, is a result of its azimuthal phase variation. In part because optical vortices carry orbital angular momentum (OAM), the study of their properties has become a rich field in physics in the last two decades with many applications, such as in optical tweezing and quantum computation.

In 2006 J.M Hickmann and collaborators at the Universidade Federal de Alagoas in Brazil [2] showed that if an optical vortex is incident on a triangular aperture, the resulting far field diffraction pattern is a triangular lattice of points that gives information on both the sign and absolute value of the topological charge in a very straightforward way. The topological charge of a vortex is an integer that says how many 2 π phase windings there are in one wavelength.

We started by recreating the work of Ref. [2] and continued by studying the diffraction of vortices by other types of apertures. The triangular and rectangular apertures were made in the Advanced Technology Lab (ATL) in the department by the EDM (Electrical Discharge Machining) method. In EDM a voltage is applied across two electrodes submersed in oil and the resulting discharge creates an aperture which matches the previosuly fabricated active electrode. The circular aperture was a commercial 1000 micron dia. pinhole. We worked with an open cavity HeNe laser and by introducing a student hair into the cavity were able to produce a wide variety of higher order HG modes. Using a standard two-cylinder-lens mode converter [1] we converted the HG modes into LG modes and tested these to determine how different topological charges affected the diffraction pattern for different apertures. Working with the triangular aperture and the set up previously described [2] we were able to reproduce the results of the Hickmann *et al.* experiment. We also attempted to see how other apertures (rectangular and circular), could be used to measure the topological charge of the vortex. With the rectangular aperture we saw a pattern that depended on the absolute value of the topological charge. Using a circular aperture an interesting pattern was seen that gave information on both the sign and absolute value of the charge. The exact nature of this pattern is still being studied, but we believe it has applications in easily measuring the topological charge of optical vortices and understanding their diffractive properties. Finally, we studied how higher topological charges affected the double slit interference pattern [3]. Although the pattern did depend on the value of the charge, this method's main usefulness is determining the sign of the charge.

This work was supported by the National Science Foundation (PHY-0851594). We would also like to thank Pete Davis (ATL) for his invaluable help in creating the apertures.

[1] M.W. Beijersbergen *et al.*, Optics Communications **96** , 123-132 (1993)

[2] J.M. Hickmann *et al.*, Phys. Rev. Lett. **105**, 053904 (2010)

[3] H.I. Sztul *et al.*, Optics Letters **31**, Issue 7, 999-1001 (2006)

Carrie Segal
Stony Brook University

Creating a stable and precisely tunable laser light source for exciting whispering gallery modes

Carrie Segal, *Stony Brook University*; MARTY COHEN, JOHN NOÉ, *Laser Teaching Center, Department of Physics & Astronomy, Stony Brook University*

The current investigation was inspired by an interest in whispering gallery mode resonators [WGMRs]. In these devices a wave travels around a circumference within a sphere or disk. The name whispering gallery is inherited from elliptical rooms in cathedrals, where a whisper that originates from one focal point can be heard with perfect clarity at the second focal point far away on the other side of the room. Whispering gallery mode resonators use the same principle except instead of sound, light undergoes total internal reflection within a circular structure as it travels around the interior.

WGMR's can achieve very high quality (Q) factors, which means that the incoming light must be precisely tuned to a specific cavity mode. A tunable diode laser would be ideal for searching for WGMR resonances but no such laser is available to us. Our alternative approach is to use an acousto-optic modulator (AOM) to shift the frequency of a stabilized single-longitudinal-mode HeNe laser. A laser of this type stable to around 15 MHz has been developed over the course of several past LTC projects. The AOM has a frequency shift range of 80 - 120 MHz and this amount can be doubled by passing the laser light through the AOM twice, using a mirror or retroreflector. Even 80 MHz is far smaller than the expected mode spacing in a small WGMR, making it quite possible that no resonance will be seen. Hopefully if several resonators are tested one will provide a detectable resonance.

We are currently creating a setup in which the double-passed frequency-shifted light from the AOM is compared with the unshifted light coming directly from the stabilized laser in a scanning Fabry-Perot resonator. The experimental challenge is to assure that the two beams enter the Fabry-Perot in precisely the same way as the frequency of the AOM is changed.

Yoonji Choe
Wellesley College

Creating and characterizing a dye laser pumped by a pulsed N_2 laser

Yoonji Choe, *Wellesley College*; JOHN NOÉ, MARTIN G. COHEN, *Laser Teaching Center, Department of Physics & Astronomy, Stony Brook University*

Dye lasers make use of organic dye molecules in solvent solutions as a gain medium and are important because they are a source of laser light precisely tunable over a relatively broad range of wavelengths. These features have made dye lasers an important tool in spectroscopy and medicine. A dye laser consists of three essential parts: an optical pump, the gain medium and an optically resonant cavity. A high pump power is required to create a population inversion in the dye solution. A pulsed laser will deliver short, high peak power pulses of very modest average power, which can create the necessary population inversion while preventing photobleaching and thermal effects in the dye.

The first step in this project was constructing the dye laser. The initial gain medium was Coumarin 500 dye diluted in ethanol at a 10^{-3} molar concentration and contained in a 5 ml quartz cuvette. The pump laser was a 337 nm nitrogen laser [Laser Science Inc. VSL 337LRF], which provides 5 ns pulses at 5 - 20 Hz and has a specified peak power of 30 kW. The pump beam was focused to a sharp horizontal line just inside the front surface of the cuvette using a quartz cylinder lens with an 18.0 cm focal length for UV light. Initially, no lasing was observed but this was later explained by the fact that the laser was only delivering 1 kW of peak power, as calculated from the measured average power and pulse width. It was subsequently discovered that an aperture attached to the front plate of the UV laser was blocking most of its output beam. Once this plate was removed, peak power increased to 7 kW and lasing was readily observed with just the parallel cuvette walls acting as the resonant cavity. Lasing stops when a glass microscope slide is inserted in the UV beam, which suggests that the threshold pump power for lasing is not much less than 7 kW.

The effect on the power and the quality of the laser beam from employing different mirror configurations has also been studied. A plane mirror and a 50 mm FL concave mirror have been used as the high reflectivity (HR) mirror. Cavity length L = 50 mm with the concave mirror was chosen to assure resonator stability. Various optics have been tested as the output coupler (OC) mirror including reflective neutral density filters, a microscope slide and a plated beam splitter. Results will be discussed.

In the coming week, we hope to continue optimizing the laser cavity as well as characterizing different dyes and dye concentrations. I also look forward to replacing the HR mirror with a diffraction grating to allow tuning the beam across the wavelength range of the dye.

Research supported by NSF Grant Phy-0851594 and the Laser Teaching Center. Thanks to Andrzej Lipski and Jonathan Sokolov for providing materials for the dye preparation and to Dr. Metcalf's lab for providing laser dyes, quartz cuvettes and a quartz cylinder lens. Last but not least, we are indebted to Prof. Metcalf for "looking under the hood" of the UV laser.

Lauren Taylor
Juniata College

Characterization of a 473 nm DPSS laser for use in oblique illumination of fluorescently tagged DNA

Lauren Taylor, *Juniata College*; JONATHAN SOKOLOV, *Garcia Center, Dept. of Materials Science & Engineering, Stony Brook University*; JOHN NOÉ, MARTIN COHEN, *Laser Teaching Center, Department of Physics & Astronomy, Stony Brook University*

This project involves characterizing a blue diode-pumped solid state (473 nm DPSS) laser for output power, polarization and beam profile. The project came about after a chance meeting with Dr. Jonathan Sokolov of the Garcia Center, whose research utilizes techniques in modern microscopy to study the structure of DNA and other polymers. Dr. Sokolov had recently purchased the DPSS laser for experiments involving oblique illumination of DNA. His proposed project was well suited to my interests, as I had become fascinated with illumination techniques and optical characteristics of microscopes through an advanced microscopy course as a sophomore at Juniata College.

Dr. Sokolov's research involves confocal imaging of fluorescently tagged double and single stranded DNA to determine tag binding orientation. DNA-specific fluorescent tags are expected to bind to the different structures in distinct orientations; this can be determined from differing responses of tags to incident polarized light. In confocal imaging (microscopy) two dimensional optical sections of a specimen are combined to form a three dimensional representation of the object. A Laser Scanning Confocal Microscope (LSCM) is equipped with one or more lasers of various wavelengths which can be used to excite fluorescently tagged specimens for imaging purposes. Unfortunately, the laser illumination system of the Garcia Center LSCM is integrated vertically into the optical train of the microscope, inhibiting the needed flexibility for proper alignment of polarized light with respect to the orientation of the DNA strands. To allow flexibility, an off-axis illumination source is necessary, provided by the separate 473 nm laser.

Our laser [1] accepts a 0 -- 5 Vdc control voltage V_c which regulates its output power. Output power as a function of V_c was measured with a calibrated power meter in 0.5 Volt steps from 0.5 to 5.0 Volts. Power was just 1.35 mW at $V_c = 0.5$ Volts and approximately doubled for each 0.5 Volt increment up to 4.0 Volts, where it leveled off at 110 mW. We later found that beam quality degrades dramatically at $V_c < 2.0$ Volts. We conclude that the laser can provide an output beam power from ~ 16 to 110 mW with acceptable beam quality.

The laser's linear polarization was next studied with a Glan-Thompson polarizer. The orientation was found to be vertical; however the maximum extinction ratio was found to be just 35:1, much poorer than the 100:1 ratio specified by the manufacturer [1].

The final and most involved set of measurements seeks to profile (determine size and shape of) the laser beam as a function of distance *z* from the laser. Several methods have been employed. In the first and simplest, the diameter (width) of the laser beam was estimated from its visual appearance at distances up to $z = 26$ meters. At the larger distances the spot was clearly seen to be elliptical (~ 50% wider than high); all of our estimates and measurements so far are confined to the horizontal plane. The visual method overestimates the true width 2 w(z) of the beam. A correction factor to account for this was obtained by comparing the estimated width at z = 8.0 meters with an actual measurement made by scanning a 1 mm square photodetector across the beam. The profile thus measured was a very close match to the Gaussian shape expected for an ideal laser mode. At $V_c = 2.0$ Volts these visual width estimates correspond to a full angular width of 0.64 milliradian (mR). According to the standard theory of

Gaussian beams, if the waist (minimum size) of the beam occurs at the face of the laser then this divergence corresponds to a waist radius of w_0 = 470 microns. Beam size near the laser was carefully measured by both the standard pinhole and razor-blade methods. These results for w_0 are 20% to 50% greater than 470 microns; the reason for this discrepancy is under investigation.

Research supported by NSF Grant PHY-0851594. We thank Suri Bandler and Ashish Sridhar for their assistance with the polarization measurement.

[1] Model DHL-B50N from Ultralasers, Inc. Toronto, Ontario, Canada. http://www.ultralasers.com.

Matthew Murray
Dickinson College

Quantum coherent control of NADH fluorescence in the free and enzyme-bound state

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Coherent control uses shaped femtosecond laser pulses to exploit the wave-like nature of quantum systems, promoting desired final states through constructive interference and limiting undesired final states through destructive interference. One application of coherent control is the selective excitation of fluorescent molecules in biological systems. Reduced nicotinamide adenine dinucleotide (NADH) is a fluorescent molecule essential to cellular metabolism. The absorbance spectrum, emission spectrum, and fluorescent lifetime of NADH are influenced by its local environment and can be used to differentiate between free NADH in solution and NADH bound to enzymes. Changes in the concentrations of free and enzyme-bound NADH have been observed in hypoxic, epileptic, and precancerous tissue samples, and advancements in the discrimination of NADH states may potentially assist in the diagnosis or treatment of these conditions and other metabolic disorders [1][2][3].

Malate dehydrogenase (MDH) is an enzyme that binds to NADH, increasing the absorbance peak of NADH by 7 nm, the emission peak by 13 nm, and the fluorescence yield by a factor of 2.2 [3]. . The shift in the emission peak of solutions containing MDH and NADH was observed with a fluorometer, confirming enzyme binding. We used an amplified titanium sapphire laser (1 KHz, 30 fs, 780 nm) and acousto-optic modulator based pulse shaper to generate pulses with a pi-phase flip in the frequency domain. We measured the two-photon fluorescence of free NADH and NADH-MDH samples as the pi-phase flip was scanned across the laser spectrum. Similar to how a damped-driven oscillator responds in phase with a driving force below the resonance frequency and out of phase above the resonance frequency, the two-photon fluorescence of free and bound NADH will be highest when the pi phase flip occurs near the center of the two photon absorption spectrum, which shifts between the two molecules.

As expected, the pi-phase scans of the NADH-MDH solutions differed from free NADH. Two pulse shapes were chosen and the fluorescence of the solutions was measured 10^6 times at each pulse shape. We constructed a histogram of the ratio between the two pulse shapes and observed that the histograms between free and bound NADH are different. The histograms remain the same at different concentration of NADH, which confirms that coherent control can be used to distinguish between NADH states. Currently, we are trying to refine this method to quantitatively measure the ratio of free and bound NADH in solutions.

This work was supported by grants from the National Science Foundation (PHY-0854922 and PHY-0851594)

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Peter Schnatz
Stony Brook University

A theoretical study of the isotopic effects on the zero-point contribution to hydrogen bonding in mineral hydrates

Peter Schnatz, PHILIP B. ALLEN, *Department of Physics & Astronomy, Stony Brook University*

Reiter et al. [1] have recently suggested that the red-shift in the zero-point motion of protons in H_2O between two phases of DNA with different levels of hydration completely accounts for the binding energy of the incorporated water molecules. Also, Nikolova and Maneva [2] have presented experimental results on the thermodynamics of nitrate-hydrates and deuterates which demonstrate that D_2O is less effective at hydrating than H_2O by up to 30%; however, the authors provide no explanation for this conclusion. After recognizing the possibility of a correlation between these two results, we explored the hypothesis that the findings in [1] could assist in predicting the binding energy of water in mineral hydrates and thus account for the shift in hydration enthalpy observed by [2].

Our focus was on true hydrates, for which the H_2O molecules that are liberated during dehydration remain in their molecular form inside the host mineral. When a mineral is hydrated the water molecules are often hydrogen-bonded to specific, energy-favorable sites within the material. The simplest binary phase diagram for the dehydration of a true hydrate shows that below the critical temperature at which the bound water molecules escape, the mineral is fully hydrated at a specific water content by weight. Mixtures lower than this water content will contain a portion of the mineral that is dehydrated, and mixtures higher than this content will have water molecules that cannot be incorporated into the mineral. At the critical temperature the H_2O molecules in the hydrated phase gain the energy required to escape from their binding sites and form water vapor.

If we limit our interests to temperatures above 300 K we can use the classical limit that would make the low-frequency vibration of the bound water molecules insensitive to isotopic substitution. Therefore, it is only the high-frequency internal vibrations (i.e. OH stretch and bending modes) that have significant zero-point contributions to the enthalpy and internal energy of the hydrate. These modes are notably responsive to isotopic substitution. Consequently, the red-shift in the bound hydrates compared to the vapor phase will be affected and a change in the critical temperature upon substitution will likely be observed.

Navrotsky [3] has developed a method to experimentally measure the enthalpy of hydration for minerals; however, this method has not been used to measure isotopic difference. In our method we consider contributions from zero-point motion, cohesive energy, and libration and hindered translational motion. From our results we hope to estimate the critical temperature shift due to isotopic substitution and determine the zero-point energy contribution to the binding energy of water in mineral hydrates.

This work was supported by a grant from the National Science Foundation (PHY-0851594)

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