ABSTRACTS OF REU FINAL REPORTS
The University of Toledo, Department of Physics &
Astronomy SUMMER 2015 (Faculty Mentor on parenthesis)

Atomic, Molecular, and Optical Physics

Kendra Bergstedt, *A Computational and Experimental Determination of F-Values of Sn II Transitions* (R. Irving and D. Ellis)

We are working to theoretically and experimentally determine f-values for some low lying transitions of Sn II, singly ionized tin. The transition probabilities are being found experimentally through beam-foil spectroscopy at the Toledo Heavy lon Accelerator (THIA). We also found oscillator strengths using the Grasp2KDev software, which utilizes the multi-configuration Dirac Hartree Fock method (MCDHF) to create relativistic electron wavefunctions. Our work is not yet completed, but some tentative results are described here.

Computational Physics

Jacob Noon, *Effects of Confinement on the Relativistic Energy Levels of Hydrogen* (R. Deck, J. Amar)

This project was directed at a relativistic calculation of the change in the energy of a hydrogenic atom produced by confinement in a spherical potential well. Although the non-relativistic analysis of this problem, based on the Schrödinger equation, had previously been completed, the relativistic calculation, based on the Dirac equation, is quite difficult and remains to be carried out.

Determination of the effect on the energy of the electron produced by confinement is important for the description of quantum dots. During the summer, a computer program was written for solving the Dirac equation subject to the additional boundary condition. But the attempt to find a proper solution of the resulting system of equations failed. Over the summer period, Jacob an extensive literature search on the problem was carried out and found that, in addition to the fact that there existed no known solution to the equations in the literature, technical problems in finding such a solution were alluded to. It is planned to continue the work on the problem during the regular academic year and summer.

Mikhael Semaan, *Submonolayer Island Nucleation and Growth for Subdiffusive Random Walkers* (J.Amar)

The breadth and variety of applications for thin film deposition, among them solar cell manufacturing and microprocessor fabrication, make the theoretical and computational study of surface growth important. While classical nucleation theory has long modeled these types of systems, it applies only to normally diffusing particles on the surface. Here, we employ kinetic Monte Carlo simulation to investigate submonolayer nucleation and growth for subdiffusive random walkers, and find that the classical theory does not hold.

Devon Shustarich, *ERoEI of modern nuclear reactors using uranium* (S. Khare)

This report examines the major components that influence the energy return on energy invested (ERoEI) of nuclear energy. The purpose is to determine which parameters impact the ERoEI the most including reactor type, the economy-wide electricity ratio, load factor, lifetime

of the reactor, distribution losses, conversion losses, milling losses, fabrication losses, thermal efficiency, heal loss factor, ore grade, burn-up, recovery rate, and tails assay. This information is gathered utilizing a software program developed by Devon Shustarich that emulates the spreadsheet utility created by the University of Sydney Australia. This software, through many automated runs, produces data relating the changing of isolated variables and the corresponding ERoEI output. The implications of these results are that the most critical components in calculating ERoEI are the burn-up, ore grade, and thermal efficiency and that nuclear energy is not sustainable.

Plasma Physics

Christopher (Alex) Robinette, *Characterization of X-ray emission during X-Pinch Shock Testing with Copper Target* (R. Irving, T. Darling)

The goal of this experiment is to sample high energy photon emissions to determine the characteristics of the pulse created by an X-Pinch configuration in the Zebra located at the Nevada Terawatt Facility, University of Nevada, Reno (UNR-NTF). Due to the nature of the pulse, speed and energy, little is known about the shape or energy distribution of the emitted photons. These factors also create issues when attempting to directly measure the electron beam produced. Using Kodak BioMax MS film in a variety of container geometries, to limit low energy background, we attempted to find the shape of the pulse as well as the energy distribution of the photons. This information allows for an indirect measurement of beam intensity and energy. As well as give more information for safety personnel regarding radiation precautions. During these tests x-ray scattering was examined closely for any anomalous behavior. Using this data we observed an unknown scattering event involving the scatter angle from an Al backscatter plate. This will be further tested and analyzed in a future experiment.

Collaborative research project conducted at The University of Toledo and Nevada Terawatt Facility at The University of Nevada, Reno. Dr. Timothy Darling is the senior scientist for this experiment at UNR-NTF and was a co-mentor of L.M. and C.R.

Hannah Salmon, *Optical Emission Spectroscopy of RF Sputter Deposition of Aluminum Doped Zinc Oxide Thin Films* (N. Podraza)

In situ optical emission spectroscopy (OES) of plasma from a radio frequency (RF) sputter deposition of aluminum-doped zinc oxide (AZO) was used to detect changes in the plasma occurring during thin film growth. The emission spectra was used to detect elemental species of the plasma by characterizing emission peak position, amplitude, and broadening assuming a Gaussian line shape. Results were benchmarked against literature. This work will enable comparison of plasma characteristics obtained from OES measurements occurred during simultaneous real time spectroscopic ellipsometry (RTSE) data acquisition. The combination of these two techniques will enable comparisons to be drawn between plasma characteristics, the resultant film properties, and the time dependence of each.

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Astrophysics

Sierra Ashley, *Changes in the Interstellar Radiation Field at High Latitudes* (A. Witt)

The interstellar radiation field (ISRF) at UV/Opt/NIR wavelengths is the integrated light

of billions of stars in the Milky Way Galaxy. Essential characteristics of the ISRF are its local energy density and its spectral energy distribution (SED). We investigated these ISRF characteristics in high-galactic latitude regions, using the emission from interstellar dust grains as probes. The color temperature of larger grains, based on the 100 *m/1* ratio, is a measure of the ISRF density, while the normalized emission intensity at mid-infrared wavelengths, produced by tiny nano-particles and large molecules in space that are heated predominantly by ultraviolet photons, reflects the relative significance of the UV component of the ISRF.

Amanda Menechella, *CO Observations of Protostellar Outflows in Orion* (T. Megeath)

<u>Context</u>. In the early stages of star formation, bipolar molecular outflows are present around the young stellar core and are still not widely understood.

<u>Aims</u>. We aim to characterize the properties of outflows of a sample of very young low-mass protostars in Orion.

<u>Methods</u>. CO 3-2 and 4-3 maps of ten Class 0 protostars were obtained using the

Atacama Pathfinder EXperiment (APEX) telescope. We estimated physical properties, such as masses and forces, for these outflows in LTE approximation.

Results. The masses and forces of the outflows were found for both the 3-2 and 4-3 transitions of CO. The outflow masses are in the range between 1.4×10^{-2} and 4.3×10^{-2} $M_{\odot}$ for CO 3-2, and in the range between 4.8×10^{-2} and 1.3×10^{-1} $M_{\odot}$ for CO 4-3. The outflow forces are in the range between 1.3×10^{-5} and 7.2×10^{-5} $M_{\odot}$ km s^{-1} yr^{-1} for CO 3-2 and in the range between 2.1×10^{-5} and 5.0×10^{-5} $M_{\odot}$ km s^{-1} yr^{-1} for CO 4-3. The outflow forces of the sources discussed in this paper are about a factor of 100 below those found for other class 0 protostars. In addition to the low outflow forces, there is no correlation between the forces and the bolometric luminosities of the sources studied in this paper.

Condensed Matter Physics

Tim Alderson, *Calculating Optical Properties Using Density Functional Theory* (S. Khare)

In the field of theoretical condensed matter physics, optical properties have recently become a relatively popular and ground-breaking topic of discussion. Using a well-known theory invented 50 years ago known as Density Functional Theory (DFT), a method of calculating optical properties has been implemented as a supplement to the experimental data that has been collected in the last century. In my research, I use a quantum-mechanical simulator known as Vienna Ab-Initio Simulation Package (VASP) to test models and calculate the optical properties to search for a more concise theory for general theoretical optics. The goal of this project is to find a general proper theory to apply to other materials and generate sets of data for comparison with experimental data. We have now reproduced some prior results from the literature for optical properties of known semi-conductors. In the future we plan to compute these properties for new materials.

Michael Bowman, *Optimization of Cu-doped ZnTe as a Backcontact Interface Layer in CdTe Solar Applications* (Y. Yan)

In order to achieve the maximum efficiency in CdS/CdTe solar cells, an efficient interface layer between the CdTe and metal cathode is necessary. In this study we investigate copper doped zinc telluride (ZnTe:Cu) as a possible interface layer for CdTe devices. In particular we examine films of zinc telluride deposited using RF magnetron sputtering at

temperatures under 300 C. We find that ZnTe:Cu films deposited at 300 ^{0}C had optimal electrical properties, such a low resistance and high carrier concentration. However, we find that higher sputtering temperatures allows the copper to diffuse at an uncontrollable rate, reducing the efficiency of the cell.

Dylan Hamilton, *Characterization of ALD Deposited Tin Oxide Buffer Layers* (Y. Yan)

SnO_2 was deposited via atomic layer deposition to serve as a buffer layer in CdTe thin film solar cells. The as-deposited film showed poor electrical properties, with carrier concentrations on the order of 10^{10}-10^{13} cm^{-3}. Significantly, it was found that annealing in an Ar ambient increased electrical and optical properties dramatically, raising the carrier concentration to 10^{18}-10^{19} cm^{-3} and the transmittance by 5-10% in the visible wavelengths. It was also found that annealing led to a polycrystalline phase as opposed to an amorphous one before annealing. The completed cell made with the buffer layer shows the need for further tuning of the carrier concentration during annealing by further exploring effects of annealing time, temperature, and oxygen content in the annealing ambient.

James McCulloch, *Stimulated Metal Whisker Growth* (D. Shvydka)

Metal whiskers are needlelike objects the can grow from grains on a metal surface. The purpose of this experiment was to stimulate metal whisker growth. Charging pre-existing whiskers and creating an electric field is theorized to stimulate their growth. To test this five samples were used. Images were taken of all samples. Then, four of the samples were irradiated in various accelerators. More images were then take of the samples. Next, before and after whisker densities were calculated from the images. An MCNP code was written to determine if whisker growth is related to the energy deposited in the sample. It was concluded that stimulated whisker growth is related to charging a sample and creating an electric field in the metal, not depositing energy into it.

David Raker, *Physics of Solar Radiation and Photovoltaic Module and System Performance* (M. Heben, R. Ellingson)

The REU project explored the application of a set of physics-based models for each stage in the process of conversion of sunlight to electricity in order to predict the output of photovoltaic systems. Modeled quantities included solar irradiance, weather, shading, factors affecting the current/voltage performance of modules, power conversion, and the final power output. The models were validated against a dataset derived from a 38 kW photovoltaic array at U. Toledo’s Wright Center for Photovoltaics.