

# Numerical Optimization of Organic Photovoltaic Cells

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## Abstract

Energy is of high demand in the 21st century and natural resources are depleting. Therefore, it is of interest to produce energy in ways that are not harmful to the environment. The process of converting the sun's light into electrical energy is a clean way to produce energy. Currently, organic photovoltaic cells (O.P.V.'s) have come into interest as they are relatively inexpensive to produce and they can be built on flexible substrates. Presently, O.P.V.'s are not efficient enough to warrant wide-scale production. In order to increase the efficiency of O.P.V.'s we have numerically modeled several O.P.V. structures. We used the First Reaction Method and the Finite Element Method in order to model the following O.P.V. structures: bulk hetero-junction, planar hetero-junction, mixed hetero-junction, and interdigitated. The research indicated that interdigitated O.P.V. structures produce significantly greater photocurrent than bulk hetero-junction and planar hetero-junction configurations.

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## In-Silico Molecular Modeling of the Inverse-Sandwich Dianion [Si<sub>6</sub>Cl<sub>14</sub>]<sup>2-</sup>

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## Abstract

Gas-phase geometry optimizations were obtained for Si<sub>6</sub>Cl<sub>12</sub> conformers and the [Si<sub>6</sub>Cl<sub>14</sub>]<sup>2-</sup> dianion at the B3LYP/6-311+G(3df) & 6-31+G(3df) level. The [Si<sub>6</sub>Cl<sub>14</sub>]<sup>2-</sup> dianion is shown to have a planar (D<sub>6h</sub>) Si<sub>6</sub> backbone whereas Si<sub>6</sub>Cl<sub>12</sub> carries a "chair" (D<sub>3d</sub>) Si<sub>6</sub> structure. Second-order Jahn-Teller distortion is proposed as the mechanism for the buckling of the Si<sub>6</sub>Cl<sub>12</sub> ring on the basis of molecular orbital and frequency calculations. The totally symmetric vibrational modes were assigned in the Raman spectra of Si<sub>6</sub>Cl<sub>12</sub> and [Si<sub>6</sub>Cl<sub>14</sub>]<sup>2-</sup> and are compared with theoretical results. A significant red shift of both Si-Si ring and Si-Cl modes was observed experimentally, and is consistent with the predicted softening of the theoretical Raman bands observed for a D<sub>3d</sub> to D<sub>6h</sub> transition of the Si<sub>6</sub> core.

# Exploration of Rotating Structures in Convective Fluids With Simple Equipment

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## Abstract

The convective behavior of rotating water has fundamental significance in geophysical applications. Here we describe a series of laboratory experiments to study convective structures in rotating fluids in ranges of Rayleigh flux number  $Ra_f$  from  $6 \times 10^4$  to  $10^7$  and of Taylor number  $Ta$  from  $5 \times 10^6$  to  $10^7$ . A transitional convective ring pattern was seen to form from interactions between the fluid spin-up, for which we determined the times of complete formation and destruction and minimum ring diameter of the centermost ring in terms of  $Ra_f$  and  $Ta$ . The ring structure evolves into an irregular vortex grid with the number density of vortices  $N \propto h^{-2}Ta^{1/2}Ra_f^{-1/6}$ , where  $h$  is the fluid depth. Using basic equipment, such as a record player, a digital camera, a dish of water, and color dye we are able to see these relationships with some degree of accuracy.

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# Effect of Longitudinal HCAL Segmentation on Electron Identification in CMS at SLHC

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## Abstract

The Compact Muon Solenoid is a general-purpose particle detector at the Large Hadron Collider. The detector currently performs a single readout of energy for each tower along the entire depth of its hadron calorimeter. Future upgrades to the detector include the segmenting of layers of the hadron calorimeter for the purpose of improving the purity of signal. We consider new algorithms for analyzing particles depositing energy into the electromagnetic and hadron calorimeters. We examine the effects of various layer segmentations and energy deposition cutoffs to determine the optimal setup for maintaining the survival of signal. Preliminary results using a dielectron simulation indicate a marked increase in signal purity using layer segmentation. Further study is in progress to give more precise quantitative results and increase background rejection.

# Optimization of Laser Parameters for Thin Silicon Wafer Dicing

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## Abstract

A design of experiments was performed to optimize: scan speed, laser power, and repetition rate for dicing thin silicon wafers. Depth of cut and debris results for single and multiple passes with the 355 nm third harmonic of a Q-switched Nd:YVO<sub>4</sub> laser are presented.

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# MML 53: A New Low-Mass, Pre-Main Sequence Eclipsing Binary in the Lupus Cloud Discovered By SuperWASP

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## Abstract

We announce the discovery of a new low-mass, pre-main sequence eclipsing binary star in the Lupus Cloud, MML 53. This is only the 6th sub-solar mass pre-main sequence eclipsing binary known. Previous observations of MML 53 found it to be a spectroscopic multiple associated with the 15-22 Myr Upper Centaurus Lupus (UCL) cluster. Here, we identify the object as an eclipsing binary for the first time through the analysis of multiple seasons of photometric time series photometry from the SuperWASP transiting planet survey, derive an accurate ephemeris for the system, and present a double-lined orbit solution based high resolution spectra from the SMARTS 1.5m echelle spectrograph. The spectra confirm MML 53 to be a triple system of young stars composed of an eclipsing binary and a stationary third component all of which show strong lithium absorption as expected for low-mass pre main sequence stars. The 2.1 d orbit of the eclipsing pair is circular, and we find the minimum masses of the eclipsing components to be  $M_1 \sin 3i = 0.94 M_\odot$  and  $M_2 \sin 3i = 0.81 M_\odot$ , with formal uncertainties of 2.0%. The systemic radial velocity from our orbit solution,  $v_\gamma = +1.00 \pm 0.33 \pm 0.81 \text{ km s}^{-1}$  (statistical and systematic), is also consistent with kinematic membership in the UCL association, and the radii of the component stars are  $\sim 30\%$  larger than expected for main sequence stars. Follow-up modeling of high cadence, multi-band light-curve data will provide precise fundamental properties of the components of the system which will ultimately be used to place constraints on theoretical models of pre-main sequence stellar evolution. This research is supported by an NSF REU grant to the Vanderbilt Physics & Astronomy Department, and by an NSF PAARE grant to Fisk University.

# Laser Crystallized a-Si with Raman Characterization

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## Abstract

With technology trends moving towards low-temperature Roll-to-Roll processing, fabrication of electrical components can be enhanced by quick and inexpensive laser processing. This presentation will report the techniques and results of processing PECVD a-Si films using the HIPPO (High Intensity Peak Power Oscillator) laser at the third harmonic (355nm). The results include crystallization using the SLS technique, dehydrogenation of a-Si:H films, and characterization of films by micro-Raman spectroscopy and 2-D Raman plots.

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# Computational Analysis of the Lipid Monolayer

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## Abstract

The lipid monolayer is studied using imaging techniques. Image analysis is done using custom routines written in Matlab. The interfacial line tension of lipid domains are calculated using capillary wave theory. Model convolution microscopy is used to simulate the monolayer and to verify analysis techniques. Other studies such as the 2D autocorrelation, temperature, and hydrocarbon chain length dependence of the phase transition are presented.

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# Construction of a Magnetic Needle Viscometer for Measuring Surface Viscosity

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## Abstract

Rheologists and biophysicists have used viscometers to measure viscosities of bulk films and their complimentary monolayers. A magnetic needle viscometer was successfully constructed, a video capture device incorporated, and the first stages of calibration completed. We have demonstrated that an MNV can be built and tested using a small budget.