



40th Semiannual Student Symposium

Monday, December 6, 2010 – Houston Science Center, Room 102

First Prize: \$300 - Second Prize: \$200 - Third Prize: \$100

CHAIRS: Profs. James K. Meen, Angela Moeller

JUDGES: Profs. John Miller, Haibing Peng, Donna Stokes

We dedicate the 40th Semiannual Student Symposium to Prof. Ki Bui Ma who was to have served as a judge.

12:55 p.m. Welcome & Introduction of Chairs & Judges: Prof. Allan J. Jacobson, Director, TcSUH

SESSION I Prof. James K. Meen, Chair

1:00 Ibrahim Kesgin, “Mechanical Striation Approach to Achieve Low AC Loss in Second Generation HTS” [*Prof. Venkat Selvamanickam, Project Leader*]

1:20 Ngozi Amuneke, “Interplay of Chemical Pressure and Spin Degrees of Freedom for the $\text{AAg}_2\text{M}[\text{VO}_4]_2$ Type of Compounds” [*Prof. Angela Moeller, Project Leader*]

1:40 Melissa Gooch, “LiFeAs: The Puzzling Stoichiometric Superconductor” [*Prof. C. W. Paul Chu, Project Leader*]

2:00 5 Minute BREAK

2:05 Buddhi Tilakaratne, “Cluster Ion Beam Induced Modifications on Polymer Surfaces” [*Prof. Wei-Kan Chu, Project Leader*]

2:25 Debtanu De, “Observation of Multiple Superconducting Gaps in $\text{Fe}_{1+y}\text{Se}_x\text{Te}_{1-x}$ Through Andreev Reflection” [*Prof. Haibing Peng, Project Leader*]

2:45 5 Minute BREAK

SESSION II Prof. Angela Moeller, Chair

2:50 Jiming Zhang, “Simulation of Temperature Evolution of Pig Muscle Treated by Magnetic Resonance Imaging Guided High Intensity Focused Ultrasound (MRgHIFU)” [*Prof. Pei Hor, Project Leader*]

3:10 Shuangqi Song, “*In Situ* Study of Electrochemical Process of Metal Nano Nuclei Formation on Single Carbon Microfiber” [*Prof. Li Sun, Project Leader*]

3:30 5 Minute BREAK

3:35 Sladjana Maric, “The Effect of Electromagnetic Properties on the Rotation of FO Portion of ATP-Synthase” [*Prof. John Miller, Project Leader*]

3:55 Guoxiong Su, “QM/MM and MD Study on a Light-Harvesting Molecular Triad” [*Prof. Margaret Cheung, Project Leader*]

4:20 Adjournment and deliberation of judges

4:30 Announcement of winners; photos of presenters, chairs and judges

ABSTRACTS

01:00 p.m. Ibrahim Kesgin, [Prof. Venkat Selvamanickam, Project Leader]

MECHANICAL STRIATION APPROACH TO ACHIEVE LOW AC LOSS IN SECOND GENERATION HTS, Ibrahim Kesgin. Striation or filamentization of coated conductors has been demonstrated as a viable way of reduction of AC losses of coated conductors. Many striation methods, such as lithography and laser ablation, were used to achieve low AC loss. The aim of this study is to develop an alternative method, which requires low cost, offers high throughput, and is readily scalable. In this method, the buffer layer is mechanically scribed to remove thin stripes of the buffer stack followed by the deposition of REBCO via Metal Organic Chemical Vapor Deposition (MOCVD) process. AC losses of striated conductors as well as those of a reference non-striated conductor were measured in AC magnetic fields normal to the conductor at various frequencies by using a pickup coil measurement technique, and at least a factor of five reduction in AC losses was obtained. Furthermore, the results were also compared with an existing theoretical model, and close agreement was found in the high field region.

01:20 p.m. Ngozi Amuneke, [Prof. Angela Moeller, Project Leader]

INTERPLAY OF CHEMICAL PRESSURE AND SPIN DEGREES OF FREEDOM FOR THE $A\text{Ag}_2\text{M}[\text{VO}_4]_2$ TYPE OF COMPOUNDS, Ngozi E. Amuneke. A series of layered compounds of the $A\text{Ag}_2\text{M}[\text{VO}_4]_2$ type of structures have been synthesized by solid state reactions. Studies on the interplay of i) chemical pressure by variation of the cation ($A^{\text{II}} = \text{Sr}, \text{Ba}$; size effects) and ii) the spin system ($M^{\text{II}} = \text{Mn}, \text{Co}, \text{Ni}, \text{Cu}$) provides further insights into structure-properties relationships which were investigated by specific heat and magnetization measurements. Spectroscopic methods have been employed to evaluate vibrational and electronic structural aspects.

01:40 p.m. Melissa Gooch, [Prof. C. W. Paul Chu, Project Leader]

LiFeAs: THE PUZZLING STOICHIOMETRIC SUPERCONDUCTOR, Melissa Gooch. LiFeAs (“111”) is an undoped stoichiometric superconductor with a $T_c = 18$ K and no magnetic ordering, but it has been suggested that its superconductivity arises from a Li deficiency. These conflicting statements prompted further investigation into the physical properties of LiFeAs. Through chemical analysis, thermoelectric power, pressure LiFeAs was systematically investigated. In conclusion LiFeAs is a chemically compressed state which is equivalent to the high pressure state of the “1111” above their critical pressure. The negative dT_c/dp found for pressure measurements would be consistent with this conclusion and would also explain the missing magnetic order.

02:00 p.m. 5 Minute BREAK

02:05 p.m. Buddhi Tilakaratne, [Prof. Wei-Kan Chu, Project Leader]

CLUSTER ION BEAM INDUCED MODIFICATIONS ON POLYMER SURFACES, Buddhi Prasanga Tilakaratne. Ion Beam irradiation of polymer materials for biological cell patterning and guiding has created great prospects in biomedical application industries. The biological cell attachment to the ion beam irradiated regions is well described through hydrophilicity of the modified polymer surface. Here, we will illustrate the monomer and cluster carbon ion modifications of polystyrene surfaces and their influence on cellular attachments on polystyrene surfaces. The energy per atom is kept constant and the fluence of the cluster ion beams is varied from $1 \times 10^{13}/\text{cm}^2$ to $1 \times 10^{16}/\text{cm}^2$, and the hydrophilicity changes were observed based on contact angle and X-ray photoelectron spectroscopy measurement techniques.

02:25 p.m. Debtanu De, [Prof. Haibing Peng, Project Leader]

OBSERVATION OF MULTIPLE SUPERCONDUCTING GAPS IN $\text{Fe}_{1+y}\text{Se}_x\text{Te}_{1-x}$ THROUGH ANDREEV REFLECTION, Debtanu De. Iron-based superconductors have been under intensive study because of the high transition temperature and the intriguing physical mechanisms involving the superconductivity and magnetic orders. Theoretical studies on the role of spin fluctuation suggest unconventional S-wave pairing and multiple superconducting (SC) gaps due to the five disjoint Fermi surfaces. However, this multiple SC-gap scenario has yet to be confirmed in experiments. Here we report the experimental observation of five SC gaps in $\text{Fe}_{1+y}\text{Se}_x\text{Te}_{1-x}$ from Andreev reflection spectra. The evolution of the multiple SC gaps is further investigated as a function of both temperature and magnetic field. For the largest SC gap, the Andreev reflection signal persists above bulk T_c , suggesting the existence of phase-incoherent Cooper pairs.

02:45 p.m. 5 Minute BREAK

02:50 p.m. Jiming Zhang, [Prof. Pei Hor, Project Leader]

SIMULATION OF TEMPERATURE EVOLUTION OF PIG MUSCLE TREATED BY MAGNETIC RESONANCE IMAGING GUIDED HIGH INTENSITY FOCUSED ULTRASOUND (MRgHIFU), J. Zhang, R. Muthupillai and P. H. Hor. MRgHIFU is clinically used for non-invasive thermal ablation of tumor tissue. The responses of tissue thermal properties to local heating will greatly affect the effectiveness of the treatment. While both tissue thermal conductivity and perfusion rate increase under hyperthermia treatments (<45°C), their behaviors in small focused volume under extreme temperature (>60°C) conditions prevalent in HIFU surgery are largely unknown. We simulate the spatio-temporal temperature distribution of pig muscle tissue *in vivo* treated by MRgHIFU using various assumptions about tissue thermal property. We find that a fast temperature dependent perfusion rate is necessary to depict the time evolution of the temperature of the entire HIFU treatment.

03:10 p.m. Shuangqi Song, [Prof. Li Sun, Project Leader]

IN SITU STUDY OF ELECTROCHEMICAL PROCESS OF METAL NANO-NUCLEI FORMATION ON SINGLE CARBON MICROFIBER, Shuangqi Song. With better understanding and control of metal layer formation on carbon surface the electrical, magnetic, thermal, interfacial and catalytic behaviors of carbon based materials can be further improved. Experiments demonstrated that controlled metal electrodeposition on single carbon microfiber can be realized. Micro-beam synchrotron x-ray diffraction and fluorescence techniques provide practical high-resolution *in situ* characterization capability to reveal the metal nuclei formation and growth processes on individual carbon microfibers with size, distribution and microstructural information.

03:30 p.m. 5 Minute BREAK

03:35 p.m. Sladjana Maric, [Prof. John H. Miller, Project Leader]

THE EFFECT OF ELECTROMAGNETIC PROPERTIES ON THE ROTATION OF FO PORTION OF ATP-SYNTHASE, Sladjana Maric. The electromagnetic properties of Fo, a subunit of rotary motor protein complex ATP-synthase, were investigated by a combined approach of molecular dynamics simulation and semi-empirical quantum chemistry calculations. A quantitative analysis of the electric field, which is hypothesized to scale with the number of c-ring proton binding sites and the proton motive force, was performed to characterize the necessary torque that rotates the FoF1-ATP synthase. This force is driven by the potential difference between the two conducting half channels through a dipolar field on the a-subunit. The results, revealing changes in electrostatic potential along cross sections of Fo due to asymmetrically protonated half-channels in the a-subunit, underpin the driving forces acting on FO.

3:55 p.m. Guoxiong Su, [Prof. Margaret Cheung, Project Leader]

QM/MM AND MD STUDY ON A LIGHT-HARVESTING MOLECULAR TRIAD, Guoxiong Su. We investigated the hydrophobic interactions of an artificial photosynthetic molecular triad in nanoconfinement in various sizes using a combined approach of QM/MM method and all-atomistic molecular dynamics simulations with explicit water models. We use the Replica Exchange Method Dynamics (REMD) to investigate the effect of solvation and confinement on the distribution of the ensemble structures and the energy landscape of triad. The relationship of the charge distribution computed from QM/MM and the radial distribution function of water molecules at the proximity of triad will be discussed. The work presented here has profound implications for future studies of the photosynthetic function of triad that provides the opportunity for the insight into the molecular device of green energy.

04:20 p.m. ADJOURNMENT AND DELIBERATION OF JUDGES

04:30 p.m. ANNOUNCEMENT OF WINNERS; PHOTOS OF SPEAKERS, CHAIRS AND JUDGES

[Note: Please meet Sue Butler and Jacqui Boulavsky by the red wall in the HSC Lobby for photos.]