

IREE REPORT

SGER: CARBON NANOMATERIAL TRANSLOCATION AND TRANSFER

-A Supplement Grant for International Research and Education in Engineering (IREE)

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ABSTRACT This report documents the NSF-IREE research activities of Michelle Reid, an undergraduate student of Physics and Electrical and Computer Engineering, and Marcus Allegood, a graduate student of Physics, and their advisor Dr. Pu-Chun Ke, conducted at Helsinki University of Technology (HUT), Finland this past summer. Supported by an IREE grant of the National Science Foundation, both students participated in research on the fate of carbon nanomaterials in biological and ecosystems systems. Using coarse-grained simulations and atomistic molecular dynamics simulations these two students investigated the binding of gallic acid with fullerene C₇₀, and the suspension of single-walled carbon nanotubes by natural organic matter. This research was advised and assisted by the Finnish hosts - Dr. Emppu Salonen, Dr. Ilpo Vattulainen, Dr. Luca Monticelli, and Mr. Jukka Maatta. Throughout this research, Michelle and Marcus learned the state-of-the-art simulation techniques and generated data which will be reported in two manuscripts (in preparation). More than the actual research, Michelle and Marcus experienced the interesting Finnish and Scandinavia cultures, promoted the American values abroad, and established friendships with the Finnish hosts. These NSF-supported IREE research and cultural activities will certainly impact on the career developments of the two students, enhance the research exchange between Clemson University and HUT, and promote the participation of underrepresented groups in science and engineering, in line with the mission statement of the NSF-IREE program.

INTRODUCTION

In 2005 the Lincoln Commission report to Congress called for U.S. universities to reach the goal of one million students studying abroad by the year 2016. This represents approximately 50% of the current US undergraduate student population. This goal is strongly supported by the National Association of State Universities and Land Grant Colleges. Congress is currently considering legislation to formally support the Lincoln Commission recommendations and declared 2006 the year of Study Abroad.

The IREE grant was awarded to the PI, Dr. Pu-Chun Ke in the Department of Physics and Astronomy at Clemson University, as a supplement grant to his SGER award entitled "Carbon Nanomaterials Translocation and Transfer". The major goal of this IREE research was to extend the SGER research in the PI's lab by examining the theoretical aspects of the solubility and bioavailability of carbon nanomaterials in aqueous solutions. Such mechanistic studies, critically lacking in the current literature, are extremely important for a better understanding of the fate of nanomaterials in biological and environmental systems.

This IREE research supported undergraduate researcher Michelle Reid (senior, Electrical and Computer Engineering and Physics), and graduate researcher Marcus Allegood (PhD student, Physics) for their research projects conducted in the Biological Physics & Soft Matter Group (BIO) at the Helsinki University of Technology (HUT) in Finland. This Finnish group has been collaborating with the PI since March 2007 and the two labs have published two joint papers on research of mutual interest. Dr. Emppu Salonen from the BIO group visited the PI's lab this March and the PI has visited the BIO group multiple times discussing research projects. The IREE grant offered a great opportunity for enhancing the research exchange between the two labs.

Michelle Reid has been a member of the PI's group since the spring of 2007. Marcus Allegood's prior REU research in the PI's lab involved measuring the solubility of C_{70} in gallic acid. Both students were well prepared in biology and computer programming. Both students were also very interested in studying abroad.

While in Finland, Michelle Reid and Marcus Allegood conducted atomistic and coarse-grained simulations on the binding of bio- and organic molecules with carbon nanostructures. Specifically, Michelle Reid constructed models for phenolic gallic acids, fullerene C_{70} , as well as a lipid bilayer to simulate the binding of gallic acid with C_{70} and their translocation across the lipid bilayer. Marcus Allegood constructed models for humic acid (a major component of organic matter in natural river sources and in agricultural soil) and a single-walled carbon nanotube. The simulations were run for tens of nanoseconds under conditions mimicking freshwater and seawater. One fundamental question the researchers addressed was how the morphology and the ionic strength of the solution affected the solubility and therefore the mobility of carbon nanomaterials discharged into the environment. Two manuscripts are in preparation and are expected to be submitted to the Journal of Physical Chemistry C and Nano Letters end of this year.

Information on the Host Laboratory: The host lab is led by Dr. Ilpo Vattulainen and Dr. Emppu Salonen. The research interests of the BIO group have been in analytical and computational modeling of biologically relevant soft matter systems. During its short period of activity the group has become a world-renowned research unit in computational modeling of biomembranes and biopolymers. Recent additions to the group's research profile are the studies of electrokinetics (i.e., the effects of applied electric fields on the dynamics of the system) in view of biomolecular manipulation, separation and characterization, and biological and environmental effects of carbon nanomaterials.

Travellers:

Michelle Reid (senior, undergraduate student, female, Electrical and Computer Engineering and Physics)

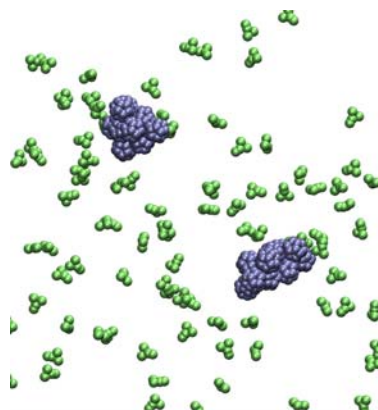
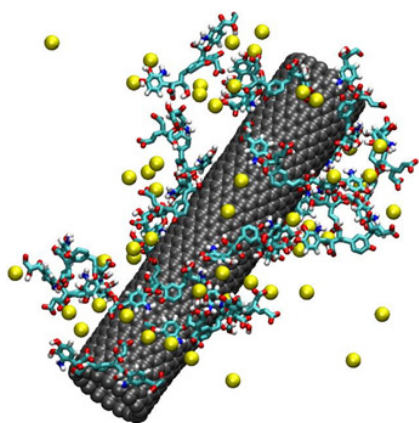
Marcus Allegood (graduate student, male, Physics)

Pu-Chun Ke (PI, assistant professor, Physics)

Dates of travel: June 4th –August 10th (Michelle Reid and Marcus Allegood), July 16th-July 21st (Pu-Chun Ke)

RESEARCH ACTIVITIES AND ACCOMPLISHMENTS OF THE INTERNATIONAL COOPERATION

- Program of research carried out during international research experience
Molecular dynamics (MD) simulations and coarse-grained simulations of gallic acid and humic acid binding with fullerene C₇₀ and carbon nanotubes
- How the work on-site is related to the work of the current NSF award
The simulations conducted by the IREE researchers facilitated interpretation of the experiment data obtained in the PI's lab at Clemson University. The overall goal of the current NSF award is to understand the impacts of man-made materials on biological and ecosystems.
- A substantive description of the general interaction between researcher and host laboratory during the international research experience
There was a positive interaction between the researchers and the host laboratory. Everyone at the host laboratory spoke English and was interested about the U.S. and was happy to talk about the culture in Finland and other countries, either ones they had been to or their home country. In the beginning of the trip when Marcus and Michelle were first learning how to do the computer simulations, most everyone made time in their schedule to help them learn how to do a desired task or help fix an error that they had encountered. Due to it being summer over in Finland and it is highly celebrated by everyone in the month of July, it became slightly more difficult to find someone to help with any problems but the host laboratory did accommodate for the researchers there and checked in periodically and communicated through email. At the end of their stay there was a small party that celebrated the researchers' time there and bid them farewell.
- Discuss the research accomplishments of student(s) during the trip
Gaining the knowledge of operating the MD simulations
Better understanding of the fate of carbon nanomaterials in the environment
- Relevant schedule, if applicable
Arriving in Helsinki on June 4th, research was started by Michelle Reid and Marcus Allegood on June 5th. The first task for them was to learn the basics behind MD simulations and using the program GROMACS. By mid-June both of them were conducting the proposed research with little aid from the researchers there. In July the PI came for a few days to talk with the heads of the lab there and to see the progress of the research. Marcus and Michelle left Helsinki, Finland on August 10th but due to the extended amount of time it takes to complete a simulation run and gather data part of the research is still ongoing in the PI's lab and at HUT.
- Two graphics that highlight the progress of the research



(Left) MD simulation of the binding of a single-walled carbon nanotube (gray) and humic acid molecules (cyan and red). (Right) Coarse-grained simulation of fullerene C₇₀ (purple) interacting with gallic acid molecules (green).

BROADER IMPACTS OF THE INTERNATIONAL COOPERATION (LIMIT: 1-1/2 PAGES)

- How the supplement award promoted diversity
The Finnish collaborators for this award aided in the experience of being aboard for Marcus and Michelle by taking care of Michelle and Marcus both in and outside of the lab. The researchers from the Finnish lab took Marcus and Michelle out to dinner several times and were especially helpful for making recommendations of events to go to or places to go. Besides living in the student dorms and being able to interact with other students and learn more about the Finnish culture, they were also able to visit some of the surrounding countries and get a broader view of the world.
- How the supplement award helps expand the original scope of the current award
The IREE research has extended the original scope of the SGER award from an experimental study to the inclusion of insightful theoretical aspects. Such combined approaches have demonstrated the most effective for describing the fate of nanomaterials in the environment.
- How the travel fosters closer future interaction between awardee institution and host institution
Both the PI's lab and the Finnish hosts and their respective institutions have benefited appreciably from this international collaboration (journal and conference publications, future proposal opportunities, students careers). This research has also opened the door for future research exchanges between the two institutions.
- How the visit has helped to enhance international perspective for the U.S. researchers. Include information on activities that increased the researcher's familiarity with foreign languages, culture, and applicable technological trends and business practices
Emerging yourself in another culture is the best way to learn through observation and personal experiences. Although Finnish is considered one of the hardest languages to learn, it was possible to learn a few common words used on a daily basis and be able to recognize a lot of words in writing that are used in signs or on menus. For understanding more of the Finnish culture, several museums located in Helsinki were visited including seeing the Suomenlinna Sea Fortress, Athenium Art Museum, and the National Museum of Finland.

DISCUSSION AND SUMMARY

- Summary of the most significant accomplishments of the international research experience
In short, the IREE grant offered a great opportunity for the students in the PI's lab to conduct their research at HUT, Finland. These students learned advanced simulation techniques which will be beneficial for the career development of these students. This summer research is expected to eventually generate 2 journal papers and multiple conference presentations. It has promoted the image and mission of the NSF abroad.
- Recommendation for "Best Practices" in future operation of the IREE Program
The grant was sufficient to cover all the expenses for the IREE student researchers, but insufficient for the PI's trip to Finland. Overall the IREE experience was excellent for all the parties involved.

ACKNOWLEDGEMENTS

The student researchers and the PI wish to acknowledge NSF grant #CBET-0736037 (program officers: Drs. Paul Bishop and Cynthia Ekstein) for supporting this IREE summer research at HUT, Finland.

BRIEF BIOGRAPHIES OF RESEARCHERS

Michelle Reid will received her BE in Electrical and Computer Engineering and a BS in Physics in May 2009. She has been a member of the PI's lab since the spring of 2007 and plans to enter graduate school after her study at Clemson University. She has co-authored a paper in the prestigious journal of Small in 2008 and is a co-author of a manuscript currently in revision with the journal of Nature Nanotechnology. Her research interest is in the area of nanoscience and nanotechnology.

Marcus Allegood received his BS in Physics from North Georgia College & State University in 2007. Prior to joining the PI's lab as a PhD student in Aug 2007, Marcus conducted summer research at Oak Ridge National Laboratory on imaging tumor cells through turbid media. This research won him a top prize at the 2008 AAAS Student Poster Competition. Marcus also conducted his REU research in the PI's lab in 2006. The research interest of Marcus is in the field of bioengineering and biophysics.