
Network for Computational Nanotechnology

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ABSTRACT: This report describes the activities of a student participant and his faculty advisor associated with a visit to the Jawaharlal Nehru Centre for Advanced Scientific Research in Bangalore, India during the Spring 2008 semester. The visit was sponsored by the US National Science Foundation's International Research Experiences for Engineers program. The primary outcomes include new research collaborations at the intersection of nanotechnology and energy, and associated computational tools to be published on nanoHUB.org, the web portal for the NSF-supported Network for Computational Nanotechnology. Other substantial outcomes include the planning and hosting of bi-lateral workshops that engage a large cross-section of researchers from the partner institutions and the development of plans to create a joint research center with a focus on nanotechnology-enabled energy solutions.

INTRODUCTION

This IREE activity was conducted under the Network for Computational Nanotechnology (PI: Mark Lundstrom, Institution: Purdue University) and involved a one-semester visit by a doctoral student to the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR). The student's advisor was co-located at JNCASR on sabbatical leave during this period as well.

The Network for Computational Nanotechnology (NCN) is a multi-institutional initiative centered at Purdue with a global reach. Its primary web portal, nanoHUB.org, provides an unparalleled platform with services for collaborative research, sharing live simulation tools online, and disseminating research methods and educational resources to a worldwide community. Almost 100,000 individuals now use the nanoHUB each year; the number is growing rapidly, and more than one-half are outside the US. The IREE program has assisted in forming new collaborations between the U.S. and Indian partners enhanced by nanoHUB's capabilities, particularly on topics at the convergence of nanotechnology and energy. Working with NCN, this initiative is expected to seed a new "Nanotechnology for Energy" area on the nanoHUB, thereby opening up a fifth major research focus and addressing an increasingly important demand for nanoHUB resources in this scientific area.

The IREE student participant, Mr. Kyle Smith, was selected on the basis of his outstanding credentials and potential for excellence in scholarly research. Mr. Smith graduated with the B.S. degree in mechanical engineering at Purdue in May 2007 as the top-ranked student of his class. He continued into the direct PhD program of Purdue's School of Mechanical Engineering in that same year and also received the prestigious NSF Graduate Fellowship award. His advisor, Prof. Timothy S. Fisher, took a sabbatical leave to JNCASR during the Spring 2008 semester, and the IREE award enabled Mr. Smith to accompany Prof. Fisher at JNCASR during this period.

JNCASR is a relatively young but already well-known multidisciplinary research institute whose mandate is to pursue and promote world-class scientific research and training at the frontiers of science and engineering. The Centre was established in 1989 by the Department of Science and Technology of the Government of India, to mark the birth centenary of Pandit Jawaharlal Nehru. The bulk of its growth has

been in the past decade. JNCASR's small size (approximately 30 faculty members, spread over several disciplines) is an advantage. Instead of being segregated in far-flung labs, chemists, physicists, biologists and engineers rub shoulders throughout the day, fostering a spirit of interdisciplinary collaboration which is one of the hallmarks of JNCASR. The intellectual atmosphere at JNCASR is further livened by a regular stream of visitors from all over the world, who contribute to spirited scientific discussions at seminars, conferences and summer schools. Researchers at the Centre are divided into six units: Chemistry and Physics of Materials, Engineering Mechanics, Evolutionary and Organismal Biology, Molecular Biology and Genetics, Theoretical Sciences, Educational Technology and Geodynamics. Though it is of course difficult to quantify scientific performance, by all numerical indications (numbers of publications, citations, grants, patents filed, etc.), science at the Centre is flourishing. In the last few years, the Centre's faculty members have published their research in some of the most prestigious scientific journals, including Nature, Nature Medicine, Science, Evolution, the Journal of the American Chemical Society, Angewandte Chemie, the Journal of Fluid Mechanics, and Physical Review Letters.

RESEARCH ACTIVITIES AND ACCOMPLISHMENTS OF THE INTERNATIONAL COOPERATION

The student was involved primarily in three primary collaborations that developed during the IREE visit as described below. All interactions were very frequent, occurring on a daily basis with engagement of the visiting student and faculty member with students, postdoctoral associates, and faculty at JNCASR.

Quasi-static Compaction of Metal Hydride Powder (International Collaborator: Prof. Meheboob Alam, JNCASR Engineering Mechanics Unit)

Metal hydrides have tremendous potential to meet on-board hydrogen storage requirements for fuel cell vehicles as set by the US DoE. Cyclic strain caused by addition and depletion of hydrogen in metal hydride beds results in brittle fracture and subsequent formation of micron-sized, faceted particles. These beds inhibit hydride formation because of poor inter-particle heat conduction that increases the bed's temperature during the exothermic hydriding reaction, but performance can be significantly improved by compaction and/or the use of thermally conductive additives. Also, reliability and durability are directly related to the mechanical properties of the additive material when metal hydride undergoes strain. To address these issues, this work involves the development of a model for generating loose configurations of metal hydride powder and for assessing the commensurate quasi-static loading characteristics. Particles in the powder are modelled by generic polyhedra with the possibility of multiple particulate species within the bed to determine the mechanical role of conducting additives. An elastic contact micro-mechanics model for particles of general shape is utilized. The numerical methods utilized to determine quasi-static equilibrium are described and exercised with particular emphasis on issues of stability and computational efficiency. A triaxial loading model is employed to simulate evolution of the solid fraction, coordination number, force network connectivity, and internal pressure as the compact is consolidated in the absence of interparticle friction. Figure 1 contains representative results from this work. Further, a public simulation tool for particle assembly and compaction is in development for deployment on nanoHUB.org and thermalHUB.org (a new NSF-sponsored project for deploying cyberinfrastructure for the heat transfer community). This work has resulted in one conference paper submission [1] and a journal paper under preparation. These modeling elements form the mechanical basis of a model that will ultimately predict the thermo-mechanical behavior of metal hydride powders and compacts for hydrogen storage.

Thermodynamics of Hydrogen Vacancies in MgH₂ from First Principles (International Collaborators: Dr. Prof. Umesh V. Waghmare and Dr. Ricardo Grau-Crespo, JNCASR, Theoretical Science Unit; Prof. N. H. de Leeuw, University College, London, Chemistry)

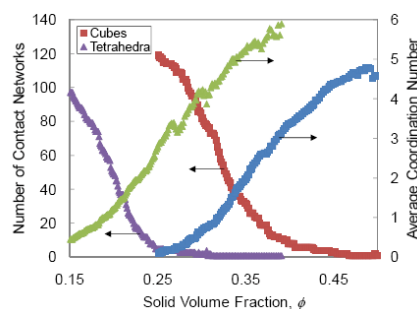


Fig. 1. Average coordination number and number of contact networks as a function of solid fraction for compaction of 125 cubes and 125 tetrahedra.

This work involves a theoretical investigation of the thermodynamics of hydrogen vacancies in magnesium hydride, using inputs from first-principles density functional theory calculations into a statistical mechanics model. We introduce a generalized method for treating site occupation disorder associated with fluctuating concentration of anions, based on a grand-canonical ensemble, which in this case is used to treat the equilibrium exchange of hydrogen between magnesium hydride MgH_2 and the gas phase of H_2 molecules. Electronic structure calculations indicate that individual neutral hydrogen vacancies leave an unpaired electron at the vacancy position, while the formation of di-vacancies is energetically more

favorable (by up to 0.4 eV per vacancy) because of the pairing of two electrons with opposite spin at the defect site. However, having determined the theoretical pressure – composition isotherms for pressures above the phase transformation point, we conclude that, contrary to a naïve expectation based on simple energetics, isolated vacancies are in fact much more abundant than their clusters at most pressures and temperatures of practical interest because of the dominance of configurational entropic effects. Figure 2 contains representative charge density distributions for mono- and di-vacancy calculations and the associated electronic density of states predictions. This work has resulted in one publication submitted for review [2], and the group intends to contribute an associated DFT simulation tool on nanoHUB.org.

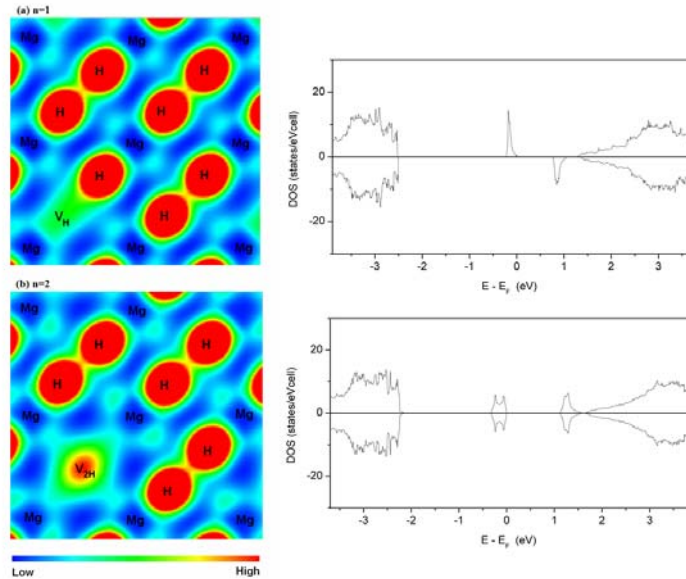


Fig. 2. Charge density distribution in the (001) plane (left) and electronic density of states (right) for a MgH_2 cell with (a) an isolated vacancy, (b) a di-vacancy cluster.

Chemical Solder for Nanoscale Contacts (International Collaborators: Prof. G.U. Kulkarni and Dr. Bhuvana Thiruvellu* JNCASR, Chemistry and Physics of Materials Unit; *Now a postdoctoral scholar at Purdue's Birck Nanotechnology Center)

This work involves the use of liquid palladium thiolate as a base material to form metallic contacts to carbon nanotubes and nanofibers. An unexpected self-assembly of these nanostructures has been demonstrated upon deposition on electron-beam-treated pads of this material. An invention disclosure and a journal paper are currently in preparation. This experimental work complements many activities of nanoHUB.org involving the simulation of contacts to nanoelements and associated device characteristics.

BROADER IMPACTS OF THE INTERNATIONAL COOPERATION

Aside from the research collaborations listed above, the participants engaged in numerous activities as summarized below.

Mr. Smith was an invited delegate to the *2008 Delhi Sustainable Development Summit*. This experience provided him with motivation for his scientific research. As a graduate student researcher in mechanical engineering, he studies study metal hydrides for use as hydrogen storage media in fuel cell vehicles, which have much promise as a sustainable transportation technology. Prior to attending the conference, Mr. Smith lacked understanding of the broader dilemma that is motivating sustainable development in the world – climate change. At the summit, his perspective on the issues and urgency of climate change was broadened, and he developed a clear picture of where his research fits into the global effort of sustainable development. Also hearing the perspectives of nontechnical players, such as politicians and media members, in sustainable development helped him tremendously to understand some of the economic mechanisms by which sustainable development can occur.

Mr. Smith also attended the 19th National & 8th Indian Society of Heat and Mass Transfer – American Society of Mechanical Engineers Heat and Mass Transfer Conference, at which he presented a paper entitled “Simulation of High-Pressure Metal Hydride Systems.” The culmination of his work at JNCASR was presented in the form of a campus-wide seminar entitled “Conduction in Metal Hydrides.” Mr. Smith also participated in the Joint India-US Workshop on Scalable Nanomaterials for Enhanced Energy Transport, Conversion, and Efficiency at JNCASR in August 2008, presenting “Thermal conductivity and packing of metal hydride powder beds.” In each of these experiences Mr. Smith received feedback from peers that greatly aided his academic professional development.

During his stay in India, Fisher participated intensively in workshops, conferences, and ongoing collaborations with faculty colleagues throughout India, and he recently became the first Adjunct Professor at ICMS. These experiences have created numerous new research directions and have led to many papers published, in review, or in preparation, as well as two joint invention disclosures. In addition to the topics described in the previous section, Fisher collaborated with Prof. CNR Rao on electronic transport in carbon nanotubes resulting in a published paper [3], with Prof. K.S. Narayan (JNCASR) on nanostructured solar cells (patent application in process), with Prof. T. Maji on metal-organic frameworks for hydrogen storage (experiments ongoing), and with Prof. S. Sampath (Indian Institute of Science) on graphene-based thermal interface materials (paper in preparation). Also, Fisher was invited to many other academic and industrial research institutions in India during and since his visit to present his research, and several of the contacts made at these institutions have led to the formation of new collaborations. These presentations include:

- T.S. Fisher, “Heterogeneous Carbon-based Nanostructures for Thermal, Electrical, and Energy Applications,” 2008 Bangalore Nano Conference, Bangalore, India, December 2008.
- T.S. Fisher, “Enhanced Energy Conversion and Storage with Nanomaterials,” Indian Institute of Technology—Madras, Chemistry Seminar Series, Chennai, India, December 2008.
- S.L. Hodson and T.S. Fisher, “Improved Thermal Conductance at Heterogeneous Carbon Nanotube Interfaces by Altering the Molecular Environment,” Molecules to Materials: New Directions—An International Conference, International Centre for Materials Science, Bangalore, India, December 2008.
- T.S. Fisher, “Overview of Energy-Related Research at the Birck Nanotechnology Center,” Vellore Institute of Technology, Vellore, India, August 2008.
- T.S. Fisher, “Carbon Nanomaterials for Old and New Energy Applications,” Joint India-US Workshop on Scalable Nanomaterials for Enhanced Energy Transport, Conversion, and Efficiency, Bangalore, India, August 2008.
- T.S. Fisher, “Enhanced Energy Conversion and Storage with Nanomaterials,” NIIST, Trivandrum, India, April 2008.
- T.S. Fisher, “Carbon-Based Nanomaterials and Devices for Enhanced Energy Transport and Conversion,” Future Directions of Advanced Materials Research: A Discussion Meeting, Shimla, India, April 2008.
- T.S. Fisher, “Heat Transfer at the Nanoscale and Some Consequences for Nanoelectronics,” IBM Technology Centre, Bangalore, India, March 2008.
- T.S. Fisher, “Engineering the Structure of Carbon Nanotubes for Biosensor Applications,” Interdisciplinary Biological Sciences Seminar Series, National Centre for Biological Sciences, Tata Institute for Fundamental Research, Bangalore, India, March 2008.
- T.S. Fisher, “Applications of Carbon Nanotubes for Enhanced Heat Transfer,” Mechanical Engineering Seminar Series, Indian Institute of Science, Bangalore, India, March 2008.
- T.S. Fisher, “Nanostructures for Enhanced Interfacial Thermal and Electrical Transport,” International Conference on Nano Science and Technology 2008 (ICONSAT 2008), Chennai, India, February 2008.
- T.S. Fisher, “Carbon Nanostructures for Enhanced Energy Conversion and Storage,” GE Global Research Technical Seminar Series, John F. Welch Technology Centre, Bangalore, India, February 2008.
- T.S. Fisher, “Enhanced Heat Transfer with Carbon Nanostructures,” Delphi Tech Centre, Bangalore, India, January 2008.

- T.S. Fisher, “Nanoscale Materials and Devices for Enhanced Energy Transport and Conversion: An Overview of the Nanoscale Transport Research Group at Purdue University,” Seminar Series, Jawaharlal Nehru Centre for Advanced Scientific Research, recording available at <http://thermalhub.org/resources/77>, January 2008.
- T.S. Fisher, “Heat Transfer Issues in Hydrogen Storage Technologies,” International Workshop on Engineering Fundamentals and Applications of Fuel Cells, Jadavpur University, Kolkata, India, January 2008.
- T.S. Fisher, “Thermal Interface Materials,” International Workshop on Thermal Design and Management in Electronics, Bangalore, India, January 2008.
- T.S. Fisher, “Free Convection Cooling of Electronics,” International Workshop on Thermal Design and Management in Electronics, Bangalore, India, January 2008.

Other broad outcomes of this IREE activity include:

- Hosting of a joint workshop between Purdue and ICMS/JNCASR on Scalable Nanomaterials for Enhanced Energy Transport, Conversion, and Efficiency (19-21 August 2008). This workshop attracted more than 100 participants, including 12 US graduate students and 13 US faculty members. The final report from the workshop is available on nanoHUB (<https://www.nanohub.org/resources/5514/>). New collaborations, including the hosting of a JNCASR student at the BNC, have already been initiated, and several joint research publications are in preparation.
- Growing cyberinfrastructure interactions between the US and India enabled by Purdue’s unique HUB technologies. The nanoHUB, a science gateway developed by the Purdue-led Network for Computational Nanotechnology, has become a major international resource for nanotechnology research, education, and collaboration. More than one-third of nanoHUB’s nearly 100,000 users reside in Asia with India being a major concentration of users. The nanoHUB currently addresses nanoelectronics, NEMS and nanofluidics, devices for medicine and biology, and nanophotonics but is seeking partnerships to expand its coverage to include nanotechnology for energy.
- A successful proposal (by Fisher, Sands, and Sharma) to NSF’s Office of International Science and Engineering (OISE-0808979), which has agreed to sponsor two bi-lateral workshops in 2009 (the first at Purdue; the second at ICMS/JNCASR) on nanoscale interface materials.
- Generation of proposals to expand these relationships including a Joint Networked Centre proposal among Purdue, JNCASR, and GE Global Research submitted to the Indo-US Science and Technology Forum in late 2008 (decision pending), and an anticipated proposal to the NSF PIRE program in 2009.
- Truly enriching cultural experiences for Mr. Smith, Prof. Fisher, his family (wife and three children). Prof. Fisher’s children attended a private school on the outskirts of Bangalore whose students were >90% Indian. His wife volunteered as a teacher at a free school that serves a slum area on the north side of the city (see <http://www.sukrupa.org/>). Meanwhile, Mr. Smith became deeply engaged in activities with JNCASR student groups and with a local church. For more information about their personal experiences, visit <http://thefishersinindia.blogspot.com/> (permission required; please send requests to tsfisher@purdue.edu).

DISCUSSION AND SUMMARY

The creation of a sustainable energy generation, storage, and distribution infrastructure represents a global grand challenge that requires massive transnational investments in the research and development of energy technologies that provide energy on the appropriate scale and timeframe with minimal impact on the environment and socio-economic systems. Ultimately, we need to capture vast amounts of dilute and intermittent, but essentially unlimited, solar energy to sustain our forecasted needs, and to scale its conversion to high power densities and readily storable forms. Nanotechnology offers the promise of addressing many challenges in the various segments of the energy industry—from biofuels to solar conversion to conservation. However, a mismatch between projected energy demand and deployment of solutions is soberingly apparent, and redoubled efforts in research and education are acutely needed. The research and education opportunities enabled by this IREE grant will ultimately facilitate discovery of

nanotechnology-enabled energy breakthroughs through technical engagements and collaborations in which the respective researchers will gain first-hand knowledge of current needs and research directions, and to take advantage of complementary expertise and facilities.

Of no less importance than new research discoveries is the need for educating and training a workforce that is capable of leading a revolution to sustainable energy globally. Of particular concern is the education of research personnel and engineering practitioners who are knowledgeable in the latest advances in nanoscience and nanotechnology, and are focused on and committed to energy-relevant applications. This skill set includes not only expansion of energy-specific educational programs for talented and motivated youth in colleges and universities at the undergraduate and graduate levels, but also the professional development of experienced researchers at the leading centers of energy research. Ultimately, it is our responsibility to invest wisely and with urgency in clean technologies that offer promise in helping to solve the energy challenge.

We are confident that this IREE activity has successfully established strong, lasting relationships among the collaborators that promise to positively and substantially affect the foregoing objectives. Some of the most significant accomplishments include:

- Initiation of a highly accomplished new doctoral student's graduate research program in an area of pressing global need—clean energy—informed by an enriching global experience.
- Establishment of new relationships that have led to numerous collaborative research projects, both for the student and faculty visitors as well as many other researchers in India and the US through joint workshops.
- Generation of new energy-related concepts and preliminary content for deployment on nanoHUB.org.
- Formation of a new cross-institutional arrangement through which one postdoctoral researcher from an underrepresented group (Ms. Bhuvana Thiruvolu) has already begun work under Prof. Fisher's supervision at Purdue.
- Generation of proposals to expand these relationships, including a Joint Networked Centre proposal among Purdue, JNCASR, and GE Global Research submitted to the Indo-US Science and Technology Forum in late 2008 (decision pending), and an anticipated proposal to the NSF PIRE program in 2009.

In summary, the IREE program was richly transformative to the student and faculty participants. This experience has profoundly impacted their current professional activities, and those of many colleagues, and will certainly continue to do so in the coming years and decades.

ACKNOWLEDGEMENTS

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BRIEF BIOGRAPHIES OF RESEARCHERS

Timothy S. Fisher received Ph.D. and B.S. degrees in Mechanical Engineering from Cornell University in 1998 and 1991, respectively. He joined the Purdue's School of Mechanical Engineering and Birck Nanotechnology Center in 2002 after several years at Vanderbilt University, and was promoted to Professor in 2007. In 2008 he was a Visiting Professor in the Chemistry and Physics of Materials Unit of the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR, Bangalore, India), and he now holds the position of Adjunct Professor in the International Centre for Materials Science at JNCASR. Prior to his graduate studies, he was employed from 1991 to 1993 as a design engineer in Motorola's Automotive and Industrial Electronics Group. His research has included efforts in simulation and measurement of nanoscale heat transfer, coupled electro-thermal effects in semiconductor and electron emission devices,

nanoscale direct energy conversion, molecular electronics, microfluidic devices, hydrogen storage, and computational methods ranging from atomistic to continuum scales. His current efforts include theoretical, computational, and experimental studies focused toward integration of nanoscale materials with bulk materials for enhancement of electrical, thermal, and mass transport properties. Applications of his work cover a broad range of areas, including nanoelectronics, vacuum electronics, thermal interface materials, convective cooling, thermal-electrical energy conversion, biosensors, and hydrogen storage. This work has also produced related studies of controlled synthesis of nanomaterials, particularly carbon nanotubes.

Kyle C. Smith was raised in Orrville, Ohio after which he pursued a B.S. in Mechanical Engineering. During his undergraduate studies he was employed by Air Products and Chemicals, Inc. as a mechanical engineering cooperative education student. After receiving a B.S.M.E. with Highest Distinction from Purdue University in 2007 he is now studying for Ph.D. at Purdue as an NSF Graduate Research Fellow. His research interests include heat conduction in solid-state hydrogen storage media, nano-scale thermal transport, and renewable energy solutions. At the Birck Nanotechnology Center and Zucrow Labs he is modeling heat conduction in metal hydrides and developing metal hydride compacts with enhanced heat conduction. He has been actively involved in undergraduate mentorship through Purdue's Summer Undergraduate Research Fellowship (SURF) program. Kyle and Prof. Timothy Fisher are actively collaborating with researchers in India (JNCASR, Bangalore) on several projects, including ab initio modeling of metal hydrides, discrete element modeling and quasi-static compression of metal hydride powders, and chemical nanosoldering.

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