Reaching and supporting the Computational Materials Science Community

Workshops & Symposia

The Materials Computation Center (MCC) supports to workshops, symposia, and meetings with funding, through organization and hosting, and by providing instruction and lecture materials.

The MCC also holds annual Summer Schools on current topics in computational materials science.

Funding new conferences helps them grow

Over 300 researchers and 150 graduate students attended the 2005 Symposia on Understanding Complex Systems.

- **Speakers introduce key concepts in the context of their discipline.**
- **Invited plenary talks are on a 'Scientific American' level.**
- **Lectures, with audio, are online.**

Year	Registered participants		
		Total talks	Days
2001	130	35	2
2002	105	30	2
2003	150	51	3
2004	396	110	4
2005	450	122	4

Understanding Complex Systems (UCS) brings together researchers from many academic disciplines and industry to stimulate cross-disciplinary research activities involving complex systems. Originated by Alfred Hübler (Physics, UIUC) in 2001, this event has grown yearly. The training of the speakers is rather diverse: Physics and Material Science, Engineering, Computer Science, Cognitive Science, Genetics and Biology, Math, Bioinformatics Physiology, Management, Medical Science, and Social Science.

Over four days, UCS 2005 had 300 researchers, including two Nobel Laureates, and 150 graduate students, who gave 122 talks. The speakers came from diverse backgrounds: 3-6 speakers are Hispanic, one plenary speaker is African-American, one plenary speaker is an American-Indian woman, and there were over a dozen other female speakers. International speakers came from Armenia, Bulgaria, Canada, Germany, Israel, Italy, Japan, and the United Kingdom.

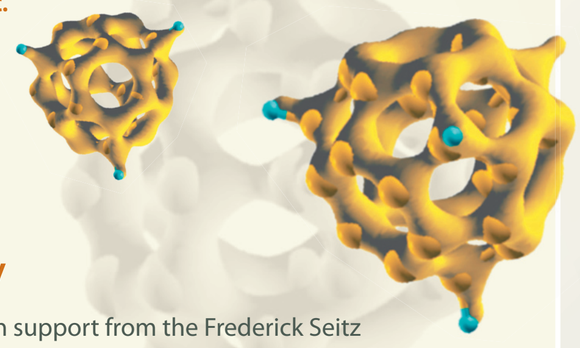
Traveling conference benefits many institutions

The annual Workshop on Recent Developments in Electronic Structure Methods brings together active participants in electronic structure theory from universities, colleges, government labs, and industrial labs from around the world. The invited presentations and contributed posters will describe new methods for computing previously inaccessible properties, breakthroughs in computational efficiency and accuracy, and novel applications of these approaches to the study of molecules, liquids, and solids.

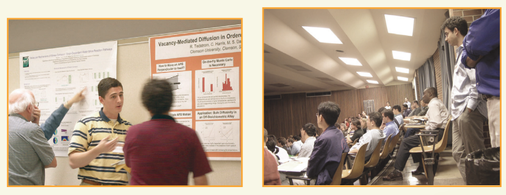
This workshop was started by David M. Ceperley and Richard M. Martin (Physics, UIUC) in 1989. In 17 years, this workshop has been hosted by 13 universities including The Ohio State University, Cornell University, Georgia Institute of Technology, University of California at Santa Barbara, St. Mary's College of Maryland, and North Carolina State University.

Each year, MCC provides seed money for the Electronic Structure Methods workshop. This funding enables wider local student participation and helps organizers gain additional support.

Above: The Thirteenth Annual Workshop on Recent Developments in Electronic Structure Algorithms (ES2001), held at Princeton University. Photo by Nicola Marzari. Below: C_{28}-derived solids, courtesy Nichols Romero, UIUC.



Hosting NSF events in the interests of the community



The NSF Division of Materials Research ITR Review, held biannually, includes presentations and poster sessions from awardees around the country. The MCC hosted the June meetings in 2002 and 2004.

With support from the Frederick Seitz Materials Research Laboratory and the National Center for Supercomputing Applications, the Materials Computation Center organizes meetings and reviews on behalf of the National Science Foundation. Through wide-scale participation, these events provide a unique, valuable snapshot of current intradisciplinary research. The MCC also maintains web archives for these events.

Materials Computation Center

University of Illinois at Urbana-Champaign • Funded by NSF DMR 03-25939

As the Computational Materials Science discipline affects all fields of science and Engineering, the Materials Computation Center (MCC) is actively developing powerful, leading-edge tools to analyze and predict the properties of materials. The MCC provides an intellectual and interactive environment for students, teachers, and researchers focused on world-class, multidisciplinary education and research in Computational Materials Science.

The MCC is headquartered and supported by facilities and services of the Frederick Seitz Materials Research Laboratory.

www.mcc.uiuc.edu

Travel Award Program

Providing research and educational networking opportunities for young scientists

The Travel Award Program supports US-based students, postdocs, and faculty to travel to workshops in Europe. Participation in international events enhances the professional development of young researchers at all levels. Participants profit from both the science presented and from new international contacts. Younger scientists from smaller institutions are particularly encouraged to apply.

Since its initiation in November 2004, 58 young scientists have applied for support and the MCC has supported 30 trips. Successful applicants came from 20 different institutions; 14% of are women and 10% are Hispanic researchers. The yearly budget is $23,000; the typical award is $800. ***www.mcc.uiuc.edu/travel***

Awardees gain career-long benefits

"This year the meeting had a total of 208 international participants, and I was honored to be one of the 34 of them that gave an oral presentation. The meeting provided a good opportunity to interact with other scientists and to learn about the work they are doing at the moment."

Oswaldo Dieguez, currently a physics and astronomy postdoctoral researcher at Rutgers University, attended the 12th International Workshop on Computational Physics & Materials Science: Total Energy & Force Methods, November 2004, held in Trieste, Italy.

"I have read articles published by many of the other attendees and had some basic familiarity with their work. This conference gave me the opportunity to directly ask them questions face to face."

Franco Capaldi attended the CECAM conference on Simulating Deformed Glasses and Melts, held September 2005 in Lyon, France. Franco's postdoctoral research at MIT focused on developing a clear connection between the underlying chemical structure and the bulk mechanical properties of polymers and serves two important purposes. It will aid engineers in the development and design of new, improved materials. It will also aid in the development of physics-based mathematical formulations that describe the connections between stress and strain in polymers. He is now an assistant professor at Drexel University.

"It gave me the chance to attend a conference that was very important for my academic formation. I can't stress enough the importance that, as an international student, these kinds of funds have since most institutions only offer grants to US citizens. Thank you."

Romelia Salomon is working towards a PhD in chemistry at the University of California, Berkeley. Her group's main research interest is applying quantum Monte Carlo methods to solve electronic structure problems. Romelia attended the Quantum Monte Carlo Tutorial Psi-K ICTP, January 2004, held in Trieste, Italy.

International cooperation brings many advantages

The Travel Award Program supports travel to workshops hosted by two established European science organizations, the Centre Européen de Calcul Atomique et Moléculaire (CECAM) and the Psi-k program of the European Science Foundation.

CECAM is a premier research institute supported by 14 organizations in Belgium, France, Germany, Greece, Italy, the Netherlands, Spain, Switzerland, and the United Kingdom. Many of the ideas of algorithms that are now commonly used in molecular simulation software have originated from workshops that CECAM has organized over the last 30 years. ***www.cecam.fr***

Psi-k focuses on the understanding of real materials and the design of new materials with improved properties and functionalities. Psi-k welcomes the whole *ab initio* community of Europe, which consists of about 2000 scientists, including students. Psi-k organizes each year approximately 17 workshops, hands-on computer courses and summer schools. ***psi-k.dl.ac.uk***

An electronic version of this poster is available at **www.mcc.uiuc.edu/research/posters.**