

**American Physical Society (APS) March 2007 meeting – Denver, CO
March 5-9, 2007**

The APS conference has an enormous turnout of scientists and researchers from all over the world. To accommodate the broad and diverse fields of physical sciences, there were at least 30 to 40 parallel sessions at one time, covering all areas of cutting-edge science and technology.

There were many outstanding invited and contributed talks delivered by world-class scientists. As a student in the field of theoretical condensed matter physics, I had the privilege to learn from the exciting talks by

- Prof. Gerbrand Ceder, Massachusetts Institute of Technology, USA

An efficient scheme to predict structures in computational materials science problems is outlined. This unusual but efficient solution can be obtained by merging ideas from heuristic and ab initio methods. By making use of the Bayesian probability network that relates the probability to find a particular crystal structure at a given composition, knowledge of both the structure and energetics is captured.

- Dr. Su-Huai Wei, National Renewable Energy Laboratory, USA
Band gap bowing coefficients in large size-mismatched II-VI alloys in the zinc-blend structure are calculated using first-principles methods. It is shown that for these systems, the bowing coefficients are large and composition-dependent. These results are in good agreement with current experiments and will aid understanding certain fundamental challenges in solar cell materials development.
- Prof. Gabor A. Somorjai, University of California, Berkeley, USA
Model surfaces from single crystals to mono-dispersed nanoparticles are investigated with state-of-the-art surface science techniques under high pressures and at liquid interfaces. Newly discovered surface phenomena include the low melting point of nanoparticles, the co-adsorption of water and hydrogen at polymer and metal surfaces. Applications of surface science expanded into nanoscience, catalysis, tribology, polymers, biointerfaces, microelectronics, energy conversion and environmental chemistry is highlighted and discussed.
- Prof. Emily Carter, Princeton University, USA
An ab initio theory has been developed over the past decade or so to describe localized correlated many-electron states in condensed matter. This embedded configuration interaction (ECI) theory is more efficient and accurate. The current version is being used to study a variety of systems/phenomena where density-functional theory (DFT) is known to fail, due either to the neglect of many-body effects or self-interaction artifacts. The Kondo effect, a long standing problem in condensed matter physics is discussed and is shown that the ECI theory is not only able to capture the physics, but also offers a new view of this phenomenon, while both DFT and finite cluster quantum chemistry calculations do not.



Entrance to APS Convention Centre in Denver

and many other fascinating talks on topics such as cyanide nanotubes, energetic materials, hydrogen storage, metal cluster chemistry and modern electronic structure theory techniques.

This experience has been a very fulfilling and enriching one for me. One of the advantages for a student to attend such an international conference is to be able to broaden one's perception of scientific research. Many conventional ideas and traditional thinking were challenged, forcing scientists to propose novel and state-of-the-art techniques and solutions. In addition, vast opportunities are created to establish new collaborative networks and to forge current on-going collaborations. I had a chance to meet up with one of our long-term collaborators, Dr. Bernard Delley, from the Paul-Scherrer-Institut in Switzerland to discuss my research findings. I was also able to establish new collaborative efforts with key scientists in my research area, namely with Dr. Jeff Grossman (UC Berkeley) and Dr. Su-Huai Wei (NREL).

Sponsorship from the Australian Institute of Physics (AIP) is greatly appreciated, without which all these will not have been possible. I would strongly recommend students like myself to partner with AIP in creating a more vibrant research environment in Australia.

-- Aloysius Soon