

**INTERNATIONAL CENTER FOR MATERIALS RESEARCH SUMMER SCHOOL ON  
FIRST PRINCIPLES CALCULATIONS FOR CONDENSED MATTER AND NANOSCIENCE**

August 21 – September 3, 2005  
University of California  
Santa Barbara, California

The International Center for Materials Research (ICMR) is organizing a residential summer school on First Principles Calculations for Condensed Matter and Nanoscience from August 21 to September 3<sup>rd</sup>. It will be directed by Michel Côté (Université de Montréal), Xavier Gonze (U. Catholique de Louvain), Nicola Spaldin (UCSB), and Gilles Zérah (Commissariat à l'énergie Atomique, Bruyères-le-Châtel).

**The structure of the summer school will be as follows:**

The school will run for two weeks, with half of the time spent in a lecture format, learning the theory and formalism needed for first-principles studies, and half of the time (the afternoons) in practical hands-on sessions in computer labs (ABINIT and OPIUM codes). During the first week, the basics of DFT total energy calculations and pseudopotential generation will be covered, followed by Density Functional Perturbation Theory for the calculations of response properties (phonons, dielectric susceptibility, elastic constants, piezoelectricity, Raman scattering, etc). During the second week, the advanced "Projector Augmented Wave" formalism will be presented, as well as methods for calculating frequency-dependent and excited state properties (the GW method, and time-dependent DFT). A poster session will be held to facilitate discussion of student research. Students will be encouraged to bring their own research problems, and to begin new collaborative projects during the workshop.

**Accommodation and Travel Information:**

Lodging and meals will be provided for the duration of the activity, beginning with dinner on Sunday, August 21st and ending with breakfast on Saturday, September 3rd. Students from the US may be reimbursed for travel expenses of up to a maximum of \$500 and students from elsewhere may be reimbursed for travel expenses of up to a maximum of \$1000 for travel expenses.

**Guidelines for submitting an application:**

We welcome applications from advanced undergraduate students, graduate students, post doctoral fellows and young researchers.

Applicants should follow application instructions presented on the ICMR website: <http://www.icmr.ucsb.edu/schools.html> For further details, please contact the ICMR Program Coordinator, Jennifer Ybarra at [Ybarra@icmr.ucsb.edu](mailto:Ybarra@icmr.ucsb.edu).

**The deadline for application is March 15, 2005.**

*ICMR Summer School on First Principles Calculations  
for Condensed Matter and Nanoscience*  
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