

ICMR Summer Program on First Principles Calculations for Condensed Matter and Nanoscience
University of California, Santa Barbara
August 21 – September 3, 2005

During this two-week program, morning sessions are lecture style, while most afternoon sessions are trainings, hands-on style. A poster session is scheduled on the evening of the third day. During the second week, four sessions of one hour are booked for the students to work on their own project and to discuss it with the instructors.

WEEK 1	
Sunday, August 21, 2005	
9:00 am to 1:00 am	Check in at the Santa Ynez Apartments (check-in open until 8/22 at 1:00 am)
5:00 pm to 7:00 pm	Dinner Reception and Registration
Monday, August 22, 2005 – Engineering Sciences Building, Room 1001	
8:00 am to 8:30 am	Continental Breakfast at Engineering Sciences Building, Room 1001
8:30 am to 8:45 am	Welcome by Tony Cheetham
8:45 am to 9:00 am	Introduction by Nicola Spaldin and other organizers
9:00 am to 10:30 am	Density Functional Theory I – Richard Martin
10:30 am to 11:00 am	Break / Discussion
11:00 am to 12:30 pm	Atoms and Pseudopotentials (basics) – Shobhana Narasimhan
12:30 pm to 2:00 pm	Lunch at the UCEN
2:00 pm to 3:00 pm	Description of the OPIUM pseudopotential package – Eric Walter and Andrew Rappe
3:00 pm to 3:30 pm	Break / Discussion
3:30 pm to 5:30 pm	Training: OPIUM (Gaviota Lab, Phelps Building, Room 1529)
5:45 pm to 7:15 pm	Dinner at De La Guerra Dining Commons
Tuesday, August 23, 2005 - Engineering Sciences Building, Room 1001	
8:15 am to 9:00 am	Continental Breakfast at Engineering Sciences Building, Room 1001
9:00 am to 10:30 am	Density Functional Theory II – Richard Martin
10:30 am to 11:00 am	Break / Discussion
11:00 am to 12:30 am	Numerical Techniques (Kohn-Sham equations, SCF, geometry) – Shobhana Narasimhan
12:30 am to 2:00 pm	Lunch at the UCEN
2:00 pm to 3:00 pm	Plane Waves / k points – Umesh Waghmare
3:00 pm to 3:30 pm	The ABINIT package and web site: How to...? Masayoshi Mikami
3:30 pm to 4:00 pm	Break / Discussion
4:00 pm to 5:30 pm	Training: ABINIT tutorials 1 – 4 (for those not familiar with these) – (Gaviota Lab, Phelps Building, Room 1529)

ICMR Summer Program on First Principles Calculations on Condensed Matter and Nanoscience
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5:45 pm to 7:15 pm	Dinner at De La Guerra Dining Commons
Wednesday, August 24, 2005 – Gaviota Lab, Phelps Building, Room 1529	
9:00 am – 3:00 pm	ABINIT tutorial 1 – 4 (for those not familiar with these) FREE DAY FOR OTHERS
12:30 pm to 2:00 pm	Lunch at the UCEN
6:00 pm to 8:00 pm	Poster Session – Dinner served at poster session
Thursday, August 25, 2005 - Engineering Sciences Building, Room 1001	
8:15 am to 9:00 am	Continental Breakfast at Engineering Sciences Building, Room 1001
9:00 am to 10:00 am	Density Functional Perturbations Theory: basics – Xavier Gonze
10:00 am to 10:15 am	Break / Discussion
10:15 am to 11:15 am	Response to atomic displacements and static electric field (zone-center phonons, Born effective charges...) - Philippe Ghosez
11:15am to 11:30 pm	Break / Discussion
11:30 am to 12:30 pm	Non Linear responses (Electro-optic effect, Raman cross-section...) – Philippe Ghosez
12:30 pm to 2:00 pm	Lunch at the UCEN
2:00 pm to 3:30 pm	Training: electric field response / zone – center phonons (Gaviota Lab, Phelps Building, Room 1529)
3:30 pm to 4:00 pm	Break / Discussion
4:00 pm to 5:30 pm	Training: non-linear responses (Gaviota Lab, Phelps Building, Room 1529)
5:45 pm to 7:15 pm	Dinner at De La Guerra Dining Commons
Friday, August 26, 2005 – Engineering Sciences Building, Room 1001	
8:15 am to 9:00 am	Continental Breakfast at Engineering Sciences Building, Room 1001
9:00 am to 10:00 am	Phonon bands, interatomic force constants and thermodynamic quantities - Umesh Waghmare
10:00 am to 10:30 am	An Introduction to Berry phases – Umesh Waghmare
10:30 am to 11:00 am	Break / Discussion
11:00 am to 12:00 pm	Finite Electric Field – Ivo Souza
12:00 pm to 12:30 pm	Parallelism – Yann Pouillon
12:30 pm to 2:00 pm	Lunch at the UCEN
2:00 pm to 3:00 pm	Training: phonon bands (Gaviota Lab, Phelps Building, Room 1529)
3:00 pm to 3:15 pm	Break / Discussion
3:15 pm to 4:15 pm	Training: electric field (Gaviota Lab, Phelps Building, Room 1529)

ICMR Summer Program on First Principles Calculations on Condensed Matter and Nanoscience
 University of California, Santa Barbara
 August 21 – September 3, 2005

4:15 pm to 4:30 pm	Break / Discussion
4:30 pm to 5:30 pm	Training: parallelism (Gaviota Lab, Phelps Building, Room 1529)
7:00 pm	Meet at the Santa Ynez Parking Lot for transportation to the El Paseo Restaurant
7:30 pm – 9:30 pm	Dinner at El Paseo Restaurant
Saturday, August 27, 2005 – Engineering Sciences Building, Room 1001	
8:15 am to 9:00 am	Continental Breakfast at Engineering Sciences Building, Room 1001
9:00 am to 10:00 am	Electron-phonon interaction – Mathieu Verstraete
10:00 am to 10:15	Break / Discussion
10:15 am to 11:15 am	Spin-polarized systems, spin-orbit coupling - Gilles Zérah
11:15 am to 11:30 am	Break / Discussion
11:30 am to 12:30 pm	Exploring the ABINIT sources – Yann Pouillon
12:30 pm to 2:00	Lunch at the De La Guerra Dining Commons
2:00 pm to 3:00 pm	Training: electron-phonon interaction (Gaviota Lab, Phelps Building, Room 1529)
3:00 pm to 3:15 pm	Break / Discussion
3:15 pm to 4:15 pm	Training: spin polarized systems, spin-orbit coupling (Gaviota Lab, Phelps Building, Room 1529)
4:15 pm to 4:30 pm	Break / Discussion
4:30 pm to 5:30 pm	Training: exploring the ABINIT sources (Gaviota Lab, Phelps Building, Room 1529)
5:45 pm to 7:15 pm	Dinner served at the De La Guerra Dining Commons during this time

ICMR Summer Program on First Principles Calculations on Condensed Matter and Nanoscience
 University of California, Santa Barbara
 August 21 – September 3, 2005

WEEK 2	
Sunday, August 28, 2005 – Free Day	
11:30 am to 1:30 pm	Lunch served at the De La Guerra Dining Commons during this time
5:45 pm to 7:15 pm	Dinner served at the De La Guerra Dining Commons during this time
12:00 pm to 5:00 pm	Optional Excursion – Santa Ynez Valley Wine Tasting Tour
Monday, August 29, 2005 – Engineering Sciences Building, Room 1001	
8:15 am to 9:00 am	Continental Breakfast at Engineering Sciences Building, Room 1001
9:00 am to 10:00 am	Wavefunction and density analysis (DOS/Bader/Angular momentum) - Michel Côté and Matthieu Verstraete
10:00 am to 10:15 am	Break / Discussion
10:15 am to 11:15 am	Projector – Augmented Wave (PAW) basics – Marc Torrent and Francois Jollet
11:15 am to 11:30 pm	Break / Discussion
11:30 pm to 12:30 pm	Project I (Gaviota Lab, Phelps Building, Room 1529)
12:30 pm to 2:00 pm	Lunch at the UCEN
2:00 pm to 3:30 pm	Training: analysis tools (Gaviota Lab, Phelps Building, Room 1529)
3:30 pm to 4:00	Break / Discussion
4:00 pm to 5:00	Project II (Gaviota Lab, Phelps Building, Room 1529)
5:45 pm to 7:15 pm	Dinner at De La Guerra Dining Commons
Tuesday, August 30, 2005 - Engineering Sciences Building, Room 1001	
8:15 am to 9:00 am	Continental Breakfast at Engineering Sciences Building, Room 1001
9:00 am to 10:00 am	PAW generator – Marc Torrent and Francois Jollet
10:00 am to 10:15 am	Break / Discussion
10:15 am to 11:15 am	The implementation of the PAW method in ABINIT – Marc Torrent and Francois Jollet
11:15 am to 11:30 am	Break / Discussion
11:30 am to 12:30 pm	Project III (Gaviota Lab, Phelps Building, Room 1529)
12:30 pm to 2:00 pm	Lunch at the UCEN
2:00 pm to 3:00 pm	Training: PAW generator (Gaviota Lab, Phelps Building, Room 1529)
3:00 pm to 3:15 pm	Break / Discussion
3:15 pm to 4:15 pm	Training: PAW calculations (Gaviota Lab, Phelps Building, Room 1529)
4:15 pm to 4:30 pm	Break / Discussion

ICMR Summer Program on First Principles Calculations on Condensed Matter and Nanoscience
 University of California, Santa Barbara
 August 21 – September 3, 2005

4:30 pm to 5:30 pm	Project IV (Gaviota Lab, Phelps Building, Room 1529)
5:45 pm to 7:15 pm	Dinner at De La Guerra Dining Commons
Wednesday, August 31, 2005 – Free Day	
11:00 pm to 2:00 pm	Lunch at the UCEN
5:45 pm to 7:15 pm	Dinner at De La Guerra Dining Commons
Thursday, September 1, 2005 - Engineering Sciences Building, Room 1001	
8:15 am to 9:00 am	Continental Breakfast at Engineering Sciences Building, Room 1001
9:00 am to 10:30 am	GW approximation: theory and implementation – Valerio Olevano
10:30 am to 11:00 am	Break / Discussion
11:00 am to 11:45 pm	Linear and non-linear optics – Sangeeta Sharma
11:45 am to 12:00 pm	Break / Discussion
12:00 pm to 12:30 pm	Advanced application I – Gilles Zérah
12:30 pm to 2:00 pm	Lunch at the UCEN
2:00 pm to 3:30 pm	Training: GW approximation (Gaviota Lab, Phelps Building, Room 1529)
3:30 pm to 4:00 pm	Break / Discussion
4:00 pm to 5:30 pm	Training: linear and non-linear optics (Gaviota Lab, Phelps Building, Room 1529)
5:45 pm to 7:15 pm	Dinner at De La Guerra Dining Commons
Friday, September 2, 2005 - Engineering Sciences Building, Room 1001	
8:15 am to 9:00 am	Continental Breakfast at Engineering Sciences Building, Room 1001
9:00 am to 10:00 am	Time-dependent density functional theory (optical response of clusters) - Xavier Gonze
10:00 am to 10:15 am	Break / Discussion
10:15 am to 11:15 am	Response to strain perturbation (elastic constants, piezoelectricity) - Don Hamann
11:15 am – 11:30 am	Break / Discussion
11:30 am to 12:00 pm	Advanced Application II – Michel Coté
12:00 pm to 12:30 pm	Advanced Application III – Matthieu Vestraete
12:30 pm to 2:00 pm	Lunch at the UCEN
2:00 pm to 3:30 pm	Training : time-dependent density functional theory (Gaviota Lab, Phelps Building, Room 1529)
3:30 pm to 4:00 pm	Break / Discussion
4:00 pm to 5:30 pm	Training : response to strain perturbation (Gaviota Lab, Phelps Building, Room 1529)

ICMR Summer Program on First Principles Calculations on Condensed Matter and Nanoscience
University of California, Santa Barbara
August 21 – September 3, 2005

	1529)
6:00 pm to 8:00 pm	Barbecue at Goleta Beach Area A
Saturday, September 3, 2005	
8:00 am to 12:00 pm	Check Out from Santa Ynez Apartments
8:15 am to 10:00 am	Continental Breakfast at the Jameson Patio at the Santa Ynez Apartments

Note: In the second week, four sessions of one hour are booked for the students to work on their own project on the basis of ABINIT and to discuss it with instructors.

Note: Meal tickets will be provided for lunch. Tickets can be used at the following UCEN restaurants: Baba's Falafal, Paterno, Romaine's, Wendy's, Nicoletti's, Coral Tree Cafe