The Abdus Salam
International Centre for Theoretical Physics

ICTP – INFM-DEMOCRITOS – ISMO - IUT School on:
Electronic-structure calculations and
their applications in materials science

25 April – 6 May 2005

Isfahan, Iran

co-sponsored by: the Italian INFM-DEMOCRITOS National Simulation Center and
the Center for International Research & Collaboration (ISMO)

FINAL PROGRAMME

Monday, 25 April

15:00 - 15:20 OPENING

15:20 - 16:20 V. HEINE
The use (and misuse) of computer simulation for atomistic understanding of materials

16:20 - 16:40 *tea break*

16:40 - 17:20 O. GULSEREN
First principles study of the thermodynamical properties of Au at normal and high pressure

17:20 - 18:00 N. MARZARI
Extended electronic functionals for constant-pressure or constant-tension simulations of nanostructures

Tuesday, 26 April

9:00 - 10:00	A. BALDERESCHI Electronic structure of materials: from bulk to surfaces and interfaces
10:00 - 10:40	S. SCANDOLO Exploring planetary centers with ab-initio molecular dynamics
10:40 - 11:00	*tea break*
11:00 - 11:40	N. MARZARI Quantum mechanical modelling of nanostructures, one Bloch at a time
11:40 - 12:20	L. REINING Electronic excitations in TDDFT and in Many-Boby Perturbation Theory: comparisons and combinations
12:20 - 13:00	A. QTEISH EXX and EXX based GW calculations of the electronic structure of semiconductors
13:00-15:00	*lunch*
15:00 - 15:40	A. BALDERESCHI Ultrathin ionic films on silver: Structural and electronic properties
15:40 - 16:20	K. ESFARJANI Charge and heat transport in quantum devices
16:20 - 16:40	*tea break*
16:40 - 17:20	S. NARASIMHAN Melting of clusters
17:20 - 18:00	P. GIANNOZZI Vibrational spectra of model chromophores

Wednesday, 27 April

9:00 - 10:00	S. BARONI Modeling the chemical reactivity of metal surfaces
10:00 - 10:40	O. GULSEREN Carbon nanotubes: functionalization and device applications
10:40 - 11:00	*tea break*

11:00 - 11:40	M. PERESSI Semiconductor-based heterostructures: Cross-sectional imaging and characterization
11:40 - 12:20	N. TIT Suitability of the II-VI semiconductors for photonic applications: Common-cation versus common-anion superlattices
12:20 - 13:00	H. AKBARZADEH Co2MnSi, a novel material for spintronic applications
13:00 - 15:00	*lunch*
15:00 - 15:40	R. GEBAUER From optical spectra to photochemistry: Some applications of time-dependent density functional theory
15:40 - 16:20	S. SCANDOLO Electrons at the surface of wide-gap insulators
16:20 - 16:40	*tea break*
16:40 - 17:20	S.M. DE GIRONCOLI Ceria as an active catalytic substrate mixed valency in density functional theory
17:20 - 18:00	V. HEINE Concluding remarks

Thursday, 28 April

Introduction to the QUANTUM-ESPRESSO package (PG)

Installation (PG)

exercises

Input-output description - Simple examples (semic.) (MP, SdG)

Graphical User Interface (GUI) (GF)

exercises

Electronic excitations in TDDFT and in Many-Boby Perturbation Theory: comparisons and combinations (LR)

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Friday, 29 April

Pseudopotentials (PG)

Self-consistency (SdG)

k-points, metals, smearing (NM)

Basic post processing and data analysis (MP)

exercises

Introduction to Surface Physics (SN)

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Monday, 2 May

Magnetism: magnetic materials, LSDA, LSDA+U (RG)

Advanced post processing - XCrysDens (GF)

exercises

EVENING SESSION: 7-8 pm
Posters

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Tuesday, 3 May

Energy derivatives: stress, forces and structural optimization, phonons (SdG)
with a talk on quasi-harmonic thermodynamics

exercises

EVENING SESSION: 7-8 pm
free with Questions/discussions with participants

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Wednesday, 4 May

Ab-Initio Molecular Dynamics (SS)

EVENING SESSION: 7-8
mini-talks from participants

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Thursday, 5 May

The Nudged Elastic Band Method (NEB): Kinetics of rare events (SB)

EVENING SESSION: 7-8 pm
free with Questions/discussions with participants

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Friday, 6 May

Free exercises - with assistance (PG and GF)