ICTP – The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy

smr1310/Final_programme

Spring College

on

Numerical Methods in

Electronic Structure Theory

7 – 25 May 2001

Co–sponsors:

- Istituto Nazionale per la Fisica della Materia (INFM), Italy
- Absoft Corporation, USA

FINAL PROGRAMME

All lectures were held in the Adriatico Guest House

– Kastler Lecture Hall –

FIRST WEEK (7 – 11 May 2001)

Monday, 7 May

8:30 – 9:15 Registration

9:15 - 9:30 Opening Ceremony

9:30 - 11:00 S. Louie, University of California at Berkeley
Electronic excitations and response functions in solids and reduced dimensional systems

11:00 - 11:30 Coffee break

11:30 - 13:00 E. Tosatti, S.I.S.S.A.The Abdus Salam I.C.T.P. Trieste
Physics of matter at extreme conditions: ultra−high pressures and temperatures, ultra−thin metal nanowires

13:00 - 15:00 Lunch break

15:00 - 16:30 S. Baroni, S.I.S.S.A, Trieste
Primer of electronic structure theory − I

16:30 - 17:00 Coffee break

17:00 - 18:30 C. Cavazzoni, CINECA, Bologna
Advanced programming techniques − I

Tuesday, 8 May

9:30 - 11:00 S. Baroni, S.I.S.S.A, Trieste
Primer of electronic structure theory − II

11:00 - 11:30 Coffee break

11:30 - 13:00 C. Cavazzoni, CINECA, Bologna
Advanced programming techniques − II

13:00 - 15:00 Lunch break

15:00 - 16:30 A. Baldereschi, Università degli Studi, Trieste
Ecole Polytechnique Federale, Lausanne
CO chemisorption on transition−metal surfaces

16:30 - 17:00 Coffee break

17:00 - 18:30 D. Vanderbilt, Rutgers University, Piscataway
Ab−initio theory of ferroelectric perovskites

Wednesday, 9 May

9:30 - 11:00 S. de Gironcoli, S.I.S.S.A, Trieste
Density functional theory, Kohn−Sham equations,
exchange−correlation functionals

11:00 - 11:30 Coffee break

11:30 - 13:00 P. Giannozzi, Princeton University
The plane−wave pseudo−potential method (PW − I)

13:00 - 15:00 Lunch break

15:00 - 18:30 S. Baroni/P. Giannozzi
Computer Laboratory. Energy bands for free electrons

Thursday, 10 May

9:30 - 11:00 D. Alfè, University College London
Numerical Linear Algebra − I (NLA − I): factorization methods

11:00 - 11:30 Coffee break

11:30 - 13:00 P. Giannozzi, Princeton University
The plane−wave pseudo−potential method (PW − II)

13:00 - 15:00 Lunch break

15:00 - 18:30 S. Baroni/D. Alfè
Computer Laboratory. Energy bands for elemental and binary semiconductor from the empirical pseudo−potential method

Friday, 11 May

9:30 - 11:00 S. de Gironcoli, S.I.S.S.A, Trieste
Brillouin−zone integration: special points and smearing techniques

11:00 - 11:30 Coffee break

11:30 - 13:00 P. Giannozzi, Princeton University
Spectral methods: the Fast Fourier Transform

13:00 - 15:00 Lunch break

15:00 - 18:30 S. Baroni/P. Giannozzi
Computer Laboratory. Calculation of the electron charge density in insulating crystals

SECOND WEEK (14 − 18 May 2001)

Monday, 14 May

9:30 - 11:00 D. Alfè, University College London

	Numerical Linear Algebra − II (NLA − II): iterative methods
11:00 - 11:30	Coffee break
11:30- 13:00	P. Giannozzi, Princeton University The non−linear Schrödinger equation: SCF cycle vs. global minimazation
13:00 - 15:00	Lunch break
15:00 - 18:30	S. Baroni/S. de Gironcoli Computer Laboratory. Calculating the Hartree and XC potentials: the SCF loop

Tuesday, 15 May

9:30 - 13:00	S. Baroni/D. Alfè Computer Laboratory. Electronic states of very large systems from iterative diagonalization
13:00 - 15:00	Lunch break
15:00 - 16:30	G. Pastore, Università degli Studi di Trieste Classical molecular dynamics
16:30 − 17:00	Break
17:00 - 18:30	A. Dal Corso, S.I.S.S.A, Trieste First derivatives of the total energy: atomic force, crystal stress, and geometry optimization

Wednesday, 16 May

9:30 - 13:00 S. Baroni/P. Giannozzi
Computer Laboratory. Calculating the self−consistent field from
constrained minimization of the electronic total
energy

13:00 - 15:00 Lunch break

15:00 - 18:30 G. Pastore, Università degli Studi di Trieste
Computer Laboratory. Classical dynamics of a Lennard−Jones fluid

Thursday, 17 May

9:30 - 13:00 S. Baroni/A. Dal Corso
Computer Laboratory. Calculating the total energies
and atomic forces

13:00 - 15:00 Lunch break

15:00 - 18:30 G. Pastore/A. Dal Corso
Computer Laboratory. Molecular dynamics with ab−initio forces

Friday, 18 May

9:30 - 11:00 S. de Gironcoli, S.I.S.S.A, Trieste

Electronic polarizability, vibrational frequencies and other second derivatives of the energy: Density−Functional Perturbation Theory

11:00 - 11:30 Coffee break

11:30 - 13:00 G. Pastore, Università degli Studi di Trieste
Ab−initio molecular dynamics: the Car−Parrinello Langragian

13:00 - 15:00 Lunch break

15:00 - 18:30 G. Pastore/D. Alfè
Computer Laboratory. Car−Parrinello ab−initio molecular dynamics.

THIRD WEEK (21 − 25 May 2001)

Monday, 21 May

10:00 - 11:00 D. Alfè, University College London
Temperature and composition of the earth's core from Ab−initio calculations

11:00 - 11:30 Break

11:30- 13:00 Computer Laboratory. Tutoring on the PWSCF computer code

Lunch break

Afternoon /evening Individual practice in the computer laboratory

Tuesday, 22 May

9:30 - 10:30 A. Dal Corso, S.I.S.S.A, Trieste

Non−local pseudo−potentials

10:30 − 11:00 Break

11:00 - 13:00 Computer Laboratory. Tutoring on the PWSCF computer code

Lunch break

15:30 − 16:30 Participant's contributions:

A. Nevidomskyy, Ivan Franko National University, Lviv

Special points method. Case of low−symmetry lattices

A. Kokalj, S.I.S.S.A., Trieste

XCrySDen: a tutorial

Wednesday, 23 May

9:30 - 10:30 M. Peressi, Università degli Studi di Trieste

Semiconductor heterostructures

10:30 − 11:00 Break

11:00 - 13:00 Computer Laboratory. Tutoring on the PWSCF computer code

Lunch break

15:00 − 16:30 Participant's contributions:

M. R. Mohammadi Zadeh, Sharif University of Technology

RE Ba2 Cu3 O7−d superconductors

S. Jalali Asadabadi, Isfahan University of Technology

Numerical investigation of three rare−Earth valence−state in the compounds SmSn3−EuSn3−GdSn3

M. Payami Shabestar, Atomic Energy Organization of Iran, Tehran

Volume change of bulk simple metals and metal clusters due to spin polarization

A. D. E. Sayede, University of Sidi−Bel−Abbes

Ab−initio Hartree−Fock study of V2O5

Thursday, 24 May

9:30 - 10:30 S. de Gironcoli, S.I.S.S.A, Trieste

Density functional perturbation theory

10:30 − 11:00 Break

11:00 - 13:00 Computer Laboratory. Tutoring on the PWSCF computer code

Lunch

15:00 − 16:30 Participant's contributions:

U. V. Waghmare, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore

Multi−scale structure and properties of materials

C. Ravi, Anna University, Chennai

Electronic structure, phase stability and elastic constants of Sc−Al compounds

G. S. Vaitheeswaran, Anna University, Chennai

Electronic structure and ground state properties of lanthanum pnictides under pressure

A. F. R. Dib, University of Tlemcen

Molecular dynamics. Beyond the microcanonical ensemble

Friday, 25 May

9:30 - 10:30 S. Baroni, S.I.S.S.A, Trieste

Medioeval dreams come true: doing alchemy by computer

10:30 − 11:00 Break

11:00 - 13:00 Computer Laboratory. Tutoring on the PWSCF computer code

Lunch break

15:00 − 16:30 Participant's contributions:

S. Goumri−Said, University of Sidi−Bel−Abbes

The behaviour of correlation functions on trans−polyacetylene polymer: quantum Monte−Carlo study

M. Verissimo Alves, Universidade Federal do Rio de Janeiro

Polarons in carbon nanotubes

S. L. Grossman, Central Michigan University, Mt. Pleasant

The origin of structure in the Raman Spectrum of Si Se2

B. Bouhafs, University of Sidi−Bel−Abbes

When using LDA and GGA? Anomalous case in III−V boron based compound

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