

November 3, Monday

Density Functional Theory for Materials Modeling

08:30-09:00

Registration and Opening Remarks

09:00-10:40

Introduction to Density Functional Theory

Coffee Break

11:00-12:30

Introduction to Density Functional Theory + Linear Algebra Use in DFT Codes

Lunch Break

14:00-15:30

Practical Sessions with Siesta

Coffee Break

16:00-17:40

Practical Sessions with Siesta

Poster Session

November 4, Tuesday

Quantum Monte Carlo Methods for Accurate Materials Simulations

08:30-10:40

Introduction to Quantum Monte Carlo

Coffee Break

11:00-12:30

Introduction to Quantum Monte Carlo + Linear Algebra use in QMC Codes

Lunch Break

14:00-15:30

Practical Sessions with TurboRVB

Coffee Break

16:00-17:40

Practical Sessions with TurboRVB

November 5, Wednesday

Many-Body Perturbation Theory and the GW Approximation

08:30-10:40

Overview of the Yambo Code and its Main Features and Performance /
Introduction to the GW Approximation

Coffee Break

11:00-12:30

Introduction to Bethe Salpeter equation / linear algebra use in MBPT

Lunch Break

14:00-15:30

Practical Sessions with Yambo

Coffee Break

16:00-17:40

Practical Sessions with Yambo

Venue Buffet

November 6, Thursday

Pushing the Boundaries of Large-Scale Simulations

Chair: Luigi Genovese

08:30-09:00

Workshop Registration and Opening Remarks

09:00-09:45

Ayako Nakata (NIMS, Tsukuba)

09:45-10:10

Laura Ratcliff (School of Chemistry, University of Bristol)

10:15-10:40

Miguel Pruneda (CINN-CSIC, Oviedo)

Coffee Break

Recent Advances in Linear Algebra Libraries for Materials Science

Chair: Edoardo Di Napoli

11:00-11:45

Toshiyuki Imamura (Riken-CCS, Kobe)

11:45-12:10

Clément Richerfort (Jülich Supercomputing Centre)

12:10-12:35

Laura Grigori (EPFL, Lausanne)

Lunch Break

Electronic Structure and Total Energy With Many-Body Methods

Chair: Daniele Varsano

14:00-14:45

Takao Kotani (Tottori University)

14:45-15:10

Maria Hellgren (IMPIC, Sorbonne Université, Paris)

15:10-15:35

Vitaly Gorelov (LSI, Ecole Polytechnique, Palaiseau)

Coffee Break

Electronic and Optical properties of innovative materials

Chair: Giacomo Giorgi

16:00-16:45

Maurizia Palummo (University of Rome Tor Vergata)

16:45-17:10

Claudio Attacalite (CINAM Marseille)

17:10-17:35

Michele Amato (LPS, Université Paris-Saclay)

17:35-18:00

Claudio Quarti (University of Mons)

Conference Dinner (just for speakers)

November 7, Friday

Modelling and Simulation of Energy Materials

Chair: Alessandro Pecchia

08:30-09:15

Azusa Muraoka (Japan Women's University)

09:15-09:40

George Volonakis (Université de Rennes)

09:40-10:05

Aran Garcia Lekue (DIPC, San Sebastian)

Coffee Break

Machine Learning for Materials Research

Chair: Pablo Ordejon

10:30-11:15

Terumasa Tadano (NIMS, Tsukuba)

11:15-11:40

Makus Holzmann (LPMMC, Université Grenoble-Alpes)

11:40-12:05

Alessandra Serva (PHENIX, Sorbonne Université)

12:05-12:50

Tomomi Shimazaki (Yokohama City University)

Lunch Break

Greens Function Methods for Spectroscopy

Chair: Michele Casula

14:00-14:45

Lucia Reining (LSI, Ecole Polytechnique, Palaiseau)

14:45-15:10

Andrea Ferretti (CRN Nano, Modena)

15:10-15:35

Valerio Olevano (Institut Néel, Grenoble)

15:35-16:00

Fabien Bruneval (CEA Saclay)

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