AGENDA

November 3 | Monday

Density Functional Theory for Materials Modeling

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

09:00-10:40

Introduction to Quantum Monte Carlo

Coffee Break

11:00-12:30

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

Lunch Break

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EuroHPC Joint Undertaking

This project received funding from the project HANAMI, funded by the European High Performance Computing Joint Undertaking (EuroHPC JU) under the European Union's Horizon Europe framework program for research and innovation.

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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

09:00-10:40
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 Salpter 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

09:00-09:45
Ayako Nakata (NIMS, Tsukuba)

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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 (IMPMC, 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)

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16:45-17:10
Claudio Attaccalite (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 Sebstian)
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 Greonoble-Alpes)
11:40-12:05
Alessandra Serva (PHENIX, Sorbonne Université)

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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
Fabien Bruneval (CEA Saclay)

15:10-15:35
Valerio Olevano (Institut Néel, Grenoble)

15:35-16:00
Andrea Ferretti (CRN Nano, Modena)

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