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

AGENDA

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
Introduction To Many-Body Perturbation Theory

Coffee Break
11:00-12:30
Introduction To Many-Body Perturbation Theory + Linear Algebra Use in GW Codes

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: TBA

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

09:45-10:10
Laura Ratcliff (School of Chemistry, University of Bristol) TBC

10:15-10:40
Miguel Pruneda (CINN-CSIC, Oviedo)

Coffee Break

Recent Advances in Linear Algebra Libraries for Materials Science
Chair: Luigi Genovese

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)

Wrap up (5 minutes)

Lunch Break

Greens Function Methods for Spectroscopy
Chair: Alessandro Pecchia

14:00-14:45
Takao Kotani (Tottori University)

14:45-15:10
Maria Hellgren (IMPMC, Sorbonne Université, Paris)

15:10-15:35
Fabien Bruneval (CEA Saclay)

Coffee Break

16:00-16:45
Lucia Reining (LSI, Ecole Polytechnique, Palaiseau)

AGENDA

16:45-17:10
Andrea Ferretti (CRN Nano, Modena)

17:10-17:35
Valerio Olevano (Institut Néel, Grenoble)

Wrap up (5 minutes)

Conference Dinner

November 7, Friday

Modelling and Simulation of Energy Materials
Chair: TBA

09:00-09:45
Azusa Muraoka (Japan Women's University)

09:45-10:10
Vitaly Gorelov (LSI, Ecole Polytechnique, Palaiseau)

10:15-10:40
Aran Garcia Lekue (DIPC, San Sebstian) TBC

Coffee Break

Machine Learning for Materials Research
Chair: Pablo Ordejon

11:00-11:45
Terumasa Tadano (NIMS, Tsukuba)

11:45-12:10
Makus Holzmann (LPMMC, Université Greonoble-Alpes)

12:10-12:35
Alessandra Serva (PHENIX, Sorbonne Université)

Wrap up (5 minutes)

AGENDA

Electronic and Optical Properties of Innovative Materials

Chair: Giacomo Giorgi

14:00-14:45

Sergei Manzhos (Tokyo Institute of Technology)

14:45-15:10

George Volonakis (Université de Rennes)

15:10-15:35

TBA

16:00-16:45

Maurizia Palummo (University of Rome Tor Vergata)

16:45-17:10

Claudio Quarti (University of Mons)

17:10-17:35

Michele Amato (LPS, Université Paris-Saclay)

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