Workshop on electronic structure methods for strong correlation: theory, computational algorithms, and codes

Łódź April 18-20 2023

Targeting Real chemical accuracy at the EXascale

DAY 1 — 18.04

Session A: Lecture 9:00-10:30
Transcorrelated Hamiltonian methods
Full Configuration Interaction Quantum Monte Carlo

Session A: Lecture 10:45-11:30
Transcorrelated Hamiltonian methods
Full Configuration Interaction Quantum Monte Carlo

Session A 11:45-13:00
Tutorial: NECI
Transcorrelated Hamiltonian methods
Full Configuration Interaction Quantum Monte Carlo

Session A 14:30-16:00
Tutorial: NECI
Transcorrelated Hamiltonian methods
Full Configuration Interaction Quantum Monte Carlo

Session B: Lecture 16:15-17:00
CIPSI: selected configuration interaction methods for ground and excited states

Session B: Lecture 17:15-18:00
CIPSI: selected configuration interaction methods for ground and excited states

DAY 2 — 19.04

Session B: Lecture 9:00-9:45
CIPSI: selected configuration interaction methods for ground and excited states

Session B 10:00-11:30
Tutorial: Quantum Package
CIPSI: selected configuration interaction methods for ground and excited states

Session B 11:45-13:00
Tutorial: Quantum Package
CIPSI: selected configuration interaction methods for ground and excited states

Session C: Lecture 14:30-15:15
Density Matrix Renormalization Group
Symmetry-Adapted Perturbation Theory for excited states

Session C: Lecture 15:30-16:15
Density Matrix Renormalization Group
Symmetry-Adapted Perturbation Theory for excited states

Session C: Lecture 16:30-17:15
Density Matrix Renormalization Group
Symmetry-Adapted Perturbation Theory for excited states

BANQUET 19:00

DAY 3 — 20.04

Session C 9:00-10:30
Tutorial: GammCor & MOLMPS
Density Matrix Renormalization Group
Symmetry-Adapted Perturbation Theory for excited states

Session C 10:45-12:00
Tutorial : GammCor & MOLMPS
Density Matrix Renormalization Group
Symmetry-Adapted Perturbation Theory for excited states

Session D: Lecture 12:15-13:00
Machine-learning potentials

Session D 14:30-15:15
Tutorial: ML
Machine-learning potentials

Session D 15:30-16:15
Tutorial: ML
Machine-learning potentials

15 minutes

1.5 hours

Lodz University of Technology
Institute of Physics
ul. Wolczanska 217/221
93-005 Lodz, Poland

Lectures and tutorials: room 0.4

Coffee and lunch: room 0.25

TUL restaurant, B9

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Łódź April 18-20 2023

Session A

Speakers and Tutors

Ali Alavi[1]
Pablo Lopez[1]
Daniel Kats[1]

Topics covered:

Transcorrelated Hamiltonian methods
Full Configuration Interaction Quantum Monte Carlo

Tutorial Code: NECI

[1]Max Planck Institute for Solid State Research, Stuttgart

Session B

Speakers and Tutors

Anthony Scemama[1]
Abdallah Ammar[2]
Pierre-Francois Loos[1]

Topics covered:

CIPSI: selected configuration interaction methods for ground and excited states

Tutorial Code: Quantum Package

[1]CNRS, Toulouse
[2]Univeristy of Toulouse, France

Session C

Speakers and Tutors

Kasia Pernal[1]
Michal Hapka[2]
Libor Veis[3]
Aleksandra Tucholska[1]

Topics covered:

Density Matrix Renormalization Group
Symmetry Adapted Perturbation Theory for excited states
Dynamic correlation energy for strongly correlated systems

Tutorial Codes: GammCor, MOLMPS

[1]Lodz University of Technology
[2]University of Warsaw
[3]J. Heyrovsky Institute of Physical Chemistry, Prague

Session D

Speakers and Tutors

Matthias Rupp[1]

Topics covered:

Introduction to machine learning potentials
Ultra-fast interpretable machine-learning potential

Tutorial Code: ML

[1]Luxembourg Institute of Science and Technology