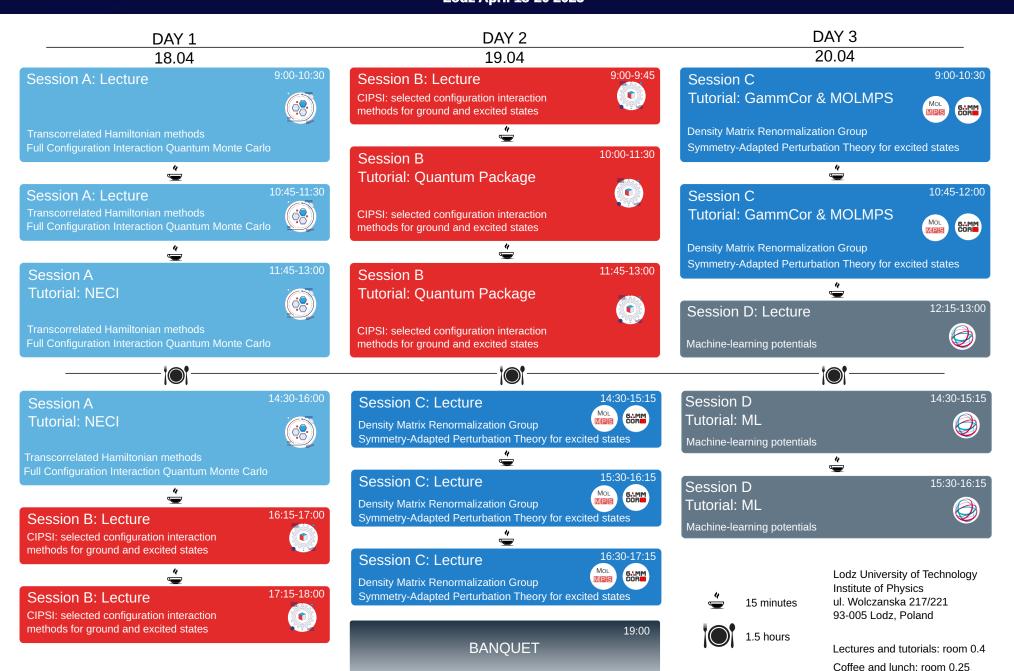


Workshop on electronic structure methods for strong correlation: theory, computational algorithms, and codes Łódź April 18-20 2023





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В

Session

Session

Speakers and Tutors

Pablo Lopez¹







Topics covered:

Full Configuration Interaction Quantum Monte Carlo

Tutorial Code: NECI

¹Max Planck Institute for Solid State Research, Stuttgart

Speakers and Tutors

Anthony Scemama¹ Emmanuel Giner² Pierre-Francois Loos¹







Topics covered:

CIPSI: selected configuration interaction methods for ground and excited states

Tutorial Code: Quantum Package

¹CNRS, Toulouse ²CNRS, Paris

Speakers and Tutors

Kasia Pernal¹ Michal Hapka² Libor Veis 3 Aleksandra Tucholska













Topics covered:

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

Tutorial Codes: GammCor, MOLMPS

Lodz University of Technology

²University of Warsaw

³ J. Heyrovsky Institute of Physical Chemistry, Prague

Speakers and Tutors Matthias Rupp 1



Topics covered:

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

Tutorial Code: ML

¹Luxembourg Institute of Science and Technology

Session