

MDanse School 2024



Monday, 4 November 2024 - Friday, 8 November 2024

ILL4

Program

Tuesday November 5th

8:45 - 9:00 -- Welcome Word by ILL Associate Director -- A. Meyer

9:00 - 10:30 -- Introduction to Density Functional Theory -- E. Rebolini

Coffee Break

11:00 - 12:30 -- Xray and Neutron Responses -- E. Farhi

Lunch at the EPN Restaurant

14:00 - 15:30 -- Hands-on: VASP and Phonopy -- P. Rozyczko

Coffee Break

16:00 - 17:30 -- Hands-on: abINS in Mantid -- S. Mukhopadhyay

Wine and Cheese - Poster Session

Wednesday November 6th

9:00 - 10:30 -- Introduction to Molecular Dynamics -- G. Kneller

Coffee Break

11:00 -12:30 -- MD Analysis -- M. Bartkowiak

Lunch at the EPN Restaurant

14:00 - 15:30 -- Hands-on: Gromacs and DLPoly -- M. Bartkowiak and M. Gonzalez

Coffee Break

16:00 - 17:30 -- Hands-on: MDANSE -- M. Bartkowiak and M. Gonzalez

Social Dinner

Thursday November 7th

9:00 - 9:30 -- Guest Lecture -- G. Kneller

9:30 - 10:30 -- Machine Learning and Molecular Dynamics -- C. Bousige

Coffee Break

11:00 -12:30 -- Introduction to Magnetism -- S. Raymond

Lunch at the EPN Restaurant

14:00 - 15:30 -- Hands-on: Takin -- T. Weber

Coffee Break

16:00 - 17:30 -- Hands-on: Takin -- T. Weber