

# MDanse School 2024



**Monday, November 4, 2024 - Friday, November 8, 2024**

**ILL4**

## Program

## Tuesday November 5th

8:00 - 8:45 -- Registration -- ILL4 Room 158

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

9:00 - 10:45 -- Introduction to Lattice Dynamics and Density Functional Theory -- E. Rebolini

*Coffee Break*

11:15 - 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

18:00 -- *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. Gonzalez

*Coffee Break*

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

19:00 -- *Social Dinner* -- Restaurant L'Epicurien

## Thursday November 7th

9:00 - 9:30 -- Quantum versus classical modeling of neutron scattering data -- 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