MDANSE 2018

Simulation of Inelastic Neutron Scattering using McStas and material dynamics models

Sept. 24th - 28th 2018
Puerto de la Cruz - Tenerife

The MDANSE 2018 is focused on the calculation of materials dynamics, e.g. dynamic structure factor $S(q,w)$ vibrational properties, using both DFT and classical MD codes. This calculation will then be forwarded to full virtual experiments of neutron scattering spectrometers in order to produce realistic simulated data, such as inelastic and quasi-elastic neutron scattering intensity. A set of representative spectrometer descriptions will be proposed to attendees, together with the so-called scattering kernels which model the neutron-matter interaction. For advanced scientists in modelling and/or neutron scattering.

Preparing data for neutron scattering virtual experiments:

- Phonons, molecular spectroscopy, magnons, structures, ...
- DFT, classical MD, ...

Inelastic neutron scattering spectrometer models with McStas

- TAS, ToF, QENS, ...

Scattering kernels (sample)

- Liquids, powders, single-crystals, ...

Assembling all bits

- Simulating both the instrument and the sample

Registration before May 31st

<http://www.isis.stfc.ac.uk/Pages/MDANSE-2018.aspx>

Organizers: E. Farhi (ILL), M.A. Gonzalez (ILL), S. Mukhopadhyay (ISIS), F. Fernandez-Alonso (ISIS), P. Willendrup (ESS/DTU), J. Taylor and T. Rod (ESS/DMSC)

<mdanse2018@ill.fr>