

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](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>



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