## MDANSE 2018

Simulation of Inelastic Neutron Scattering using McStas and material dynamics models Sept. 24<sup>th</sup> - 28<sup>th</sup> 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>

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