



Neutrons and Simulations Joint Workshop

24th October 2025

Meeting room 1&2, Research Complex at Harwell, Rutherford Appleton Laboratory,
Harwell Campus

10:00	<u>Registration Opens & Coffee</u>	Foyer Research Complex at Harwell (Building R92)
Session 1		MR 1&2, Research Complex at Harwell (Building R92)
10.30 -10.40	Welcome & Introduction	Dr. Sarah Rogers, ISIS Neutron and Muon Source
10.40 -10.55	Prof. Richard Catlow, Cardiff/UCL	Synergy between neutrons and modelling
10.55 -11:20	Dr. Ian Silverwood, ISIS Neutron and Muon Source	Neutron fundamentals
11.20 -11:45	Prof. Tom Keal, STFC Scientific Computing - <i>virtually</i>	Hybrid QM/MM simulations for catalysis
11:45 -12:10	Dr. Marta Falkowska, University of Manchester	Total Neutron Scattering of Confined Fluids: Structure Beyond the Data
12:10 -13:10	LUNCH FOYER (R92)	
	12:55- 13:10 Tour of ISIS Neutron and Muon Source	
Session 2		MR 1&2, Research Complex at Harwell (Building R92)
13:15-13:40	Dr. Adam Jackson, STFC Scientific Computing	Simulated experiments from phonon calculations: software tools
13:40-14:05	Dr. Arunabhram Chutia, Lincoln	Probing the interactions of C ₆ H ₆ +2n molecules on the Ni(111) surface using vdW-DFT and INS
14:05-14:30	Dr. Maciej Bartkowiak, ISIS	Molecular dynamics analysis for neutron users: recent changes in MDANSE
14:30- 14:55	COFFEE BREAK	Foyer, Research Complex at Harwell
15:00-15:25	Dr. Alexander O'Malley, Bath	Effectively combining quasielastic neutron scattering and molecular dynamics simulations in the study of catalysts
15:25-15:45	Mr. Lewis Waller, Southampton	Multiphysics Modelling of Electrochemical Reactors: Bridging Experiment and Simulation
15:45-15:55	Dr. Ian Silverwood, ISIS Neutron and Muon Source	Close and next steps