

Surfln Workshop: Atomistic Insights into Processes at Minerals and Materials Surfaces and Interfaces

Workshop Dates: Mon, 17 June 2019, 12:00 – 17:00

Location: Joseph Priestley South Building, Room JP2/18, Department of Chemical Sciences, School of Applied Sciences, University of Huddersfield, Queensgate, Huddersfield, HD1 3DH (Building 24 on the map:
www.hud.ac.uk/media/assets/document/maps/CampusMap.pdf)

Sponsors: CCP5 www.ccp5.ac.uk

Organisers: Marco Molinari & David J. Cooke & Samuel Moxon (University of Huddersfield)

Posters

Dr Helen Duncan (UCL, UK) – SAINT: The Surface and Interface Toolkit

Emile Durant (University of Liverpool) – A Computational Study of Tip Induced Formaldehyde Flipping on the Cu(110) Surface

Roger Thornton (University of Huddersfield) – Development of interatomic potentials for modelling uranyl compounds

Alexander Garrett (University of Manchester) – Prediction of coherent Cu nanoprecipitate geometries using particle swarm optimisation (PSO)

Joseph Flitcroft (University of Huddersfield) - Cuboidal Ceria Nanoparticles: Control of the {111}/{110} Surface Ratio

Samuel Moxon (University of Huddersfield) – The interaction of CO₂ with surfaces of PuO₂

Joshua Tse (University of Huddersfield) – The interaction of Graphene on Strontium Titanate Surfaces

Haider Farouq (University of Bradford) - The interaction of Natural Organic Matter at the Aqueous Graphene and Rutile Interfaces: The Environmental Effect of Manufactured Nanomaterials.

Nicodemo Di Pasquale (University of Leicester) – Calculation of Surface Free Energy in Mannitol Crystals Through Cleaving