

## SurfIn 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](http://www.hud.ac.uk/media/assets/document/maps/CampusMap.pdf))

**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 CO<sub>2</sub> with surfaces of PuO<sub>2</sub>

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

Aneesa Ahmad (University of Sheffield) – Adsorption of Small Organic Molecules onto the alpha-Al<sub>2</sub>O<sub>3</sub> (0001) Surface: A Computational Study

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