ScotCHEM 2020 Computational Chemistry Virtual Symposium

Wednesday 26th August 2020

Session 1

Welcome and opening remarks (09:50—10:00)

10:00—10:30	**Dr James McDonagh**	IBM Research Group	*Parameterization and automation of coarse-grained simulations for industrial chemical formulation.*
10:30—11:00	**Dr Laia Vila-Nadal**	University of Glasgow	*POMzites a roadmap for inverse design in metal oxide chemistry.*
11:00—11:30	**Jonathan Colburn**	University of St Andrews	*Quantifying Electrostatic Preorganisation in Heme Peroxidase Enzymes with QM/MM.*
11:30—12:00	**Arron Burnage**	Heriot-Watt University	*Mechanistic Study of the Room Temperature Acceptorless Dehydrogenation of an Isobutane σ-Complex in the Solid-State.*

Lunch (12:00—13:00)

Session 2

13:00—13:30	**Dr Oliver Henrich**	University of Strathclyde	*Coarse-Grained Modelling of DNA-Based Hydrogels and DNA Supercoiling.*
13:30—14:00	**Dr Daniel Dawson**	University of St Andrews	*Computational Insights into the Extensively Disordered GaPO-34A Structure.*
14:00—14:30	**Dr Xiang Sheng**	Stockholm University	*Modeling Enzymatic Enantioselectivity using Quantum Chemical Methodology.*
14:30—15:00	**Dr Rafel Szabla**	University of Edinburgh	*Modelling reactions involving UV-induced electron transfer in DNA.*

Break (15:00—15:30)

Session 3

Plenary Speaker

15:30—16:30	**Prof Adrian Roitberg**	University of Florida	*Is Quantum Chemistry Amenable for Machine Learning? Are the Computers Coming for Our Jobs?*

Poster prizes and closing remarks (16:30—16:45)