South West Computational Chemistry Meeting

Wednesday 21st November 2018, University of Bath

Chancellors Building, Room 2.6

13:00 – 13:10	**WELCOME**
13:10 – 13:30	*Intrinsic non-stoichiometry in lithium conducting garnets* Alex Squires, University of Bath
13:30 – 13:50	*The mechanical properties of graphene nanoribbons* Mat Tolladay, University of Bristol
13:50 – 14:10	*Digital Filtering Hamiltonian Monte Carlo (DFHMC) - Frequency-directed acceleration of classical rare events sampling* Khaled Abdel-Maksoud, University of Southampton
14:10 – 14:30	*Computational QM/MM and AIMD studies of the Methanol to Hydrocarbons process on zeolites H-Y and H-ZSM-5* Stefan Nastase, Cardiff University
14:30 – 14:50	*Do radical pair reactions act as quantum measurements?* Thomas Fay, University of Oxford
14:50 – 15:15	**COFFEE BREAK**
15:15 – 15:35	*Machine-Learnt Fragment-Based Energies for Crystal Structure Prediction* David McDonagh, University of Southampton
15:35 – 15:55	*Au-Pd Alloy Catalysts for the Oxidation of Organic Compounds* Ali Nasrallah, Cardiff University
15:55 – 16:15	*Investigating enzyme dynamics and catalysis by simulation* Mike Connolly, University of Bristol
16:15 – 16:35	*Modelling the Interfaces of Fluorite Structured Oxides* Adam Symmington, University of Bath
17:00 –	**POSTER SESSION** (1 South)