ScotCHEM 2016 Programme

Tuesday 14th June 2016

Lecture Theatre A, JCMB, University of Edinburgh

09:30 Registration

10:25 Welcome and opening remarks

Session 1 (Chair: Dr Philip J. Camp)

10:30 Dr Paola Carbone (Manchester) *Plenary talk: Multiscale modelling of polymer aggregates*

11:20 Mr Jiabo Le (Aberdeen) *Determining potential of zero charge from density functional theory based molecular dynamics*

11:50 Mr Tomasz K. Piskorz (Delft and Strathclyde) *Self-assembly of functionalized long-chain alkanes on graphite*

12:10 Dr Andy Turner (EPCC) *Profiling parallel software use on UK national supercomputing services*

12:20 Lunch

Session 2 (Chair: Dr Julien Michel)

13:20 Ms Rachel E. Skyner (St Andrews) *Using the Cambridge Structural Database (CSD) to probe solubility and its prediction*

13:50 Dr Jordi Juárez-Jiménez (Edinburgh) *Combining accelerated molecular dynamics and Markov state models to disclose hidden protein states: Towards the development of selective cyclophilin inhibitors*

14:10 Dr Therese Bergendahl (Edinburgh) *Computational modelling of protein complexes – Using structure and stability to inform genetic disease variants*

14:30 Dr David M. Rogers (Edinburgh) *Quantum chemistry calculations on halogenated benzenes*

15:00 Tea and coffee

Session 3 (Chair: Prof. Stuart A. Macgregor)

15:30 Mr Nicholas Beattie (Heriot-Watt) *Computational Studies into the dehydrocoupling of amine-boranes*

15:50 Ms Katie J. Emery (Strathclyde) *Mechanistic Investigation into cyclisation's involving radical intermediates*

16:10 Mr Innis Carson (Edinburgh) *Computational modelling techniques for the design of solvent extractants for metals*

16:30 Prof. Rob Deeth (Edinburgh and Warwick) *Copper acetate and related species: Complex complexes for MOF secondary building units*

17:00 Flash presentations presented by the NSCCS

17:00 Posters and drinks reception