Meeting Schedule

Sunday 15 March

15.00	**Registration opens in the Students Union Building**
19.00 - 20.00	*Dinner and welcome*
20.00 onwards	*Informal 'mixer' event in the Rootes Bar*

Monday 16 March

9.00 - 10.00	**Keynote lecture 1: Prof. Cecilia Clementi** *Advanced Sampling with Diffusion Coordinates*
10.00 - 10.30	Prof. Jonathan Hirst *Electronic circular dichroism and 2D-ultraviolet spectroscopy of proteins*
10.30 - 11.00	*Refreshments*
11.00 - 11.30	Prof. Ali Alavi *Recent developments in FCIQMC*
11.30 - 12.00	Dr. Gareth Shannon *HECBioSim: Who we are and how we support the biomolecular simulation community*
12.00 - 12.30	Prof. David Manolopoulos *Semiclassical spin dynamics and avian magnetoreception*
12.30 - 14.00	*Lunch*
14.00 - 14.30	Prof. Jochen Blumberger *Towards a molecular-scale understanding of charge transfer processes in material science and biology*
14.30 - 15.30	**Keynote lecture 2: Prof. Sharon Hammes-Schiffer** *Proton-Coupled Electron Transfer in Catalysis and Energy Conversion*
15.30 - 16.00	*Refreshments*
16.00 - 16.30	Prof. Fred Manby *Quantum embedding*
16.30 - 17.00	Prof. Ian Williams *Isotope Effect Calculations in the Supramolecular Age*
17.00 - 17.30	Dr. Robert Paton *Refining the Rules for Ring Closure: Computations and Organocatalytic Cyclizations*
18.30 - 19.30	*Dinner*
19.30 - 22.00	Poster session on Science Concourse

Tuesday 17 March

9.00 - 10.00	***Warwick Materials GRP symposium*** **Keynote lecture 3: Prof. George Schatz** *Modeling the self-assembly of DNA- and peptide-based optical materials*
10.00 - 10.30	Dr. Juan Arago March *Exciton transport in organic crystals: The role of the dynamic disorder in coherent and incoherent regimes*
10.30 - 11.00	*Refreshments*
11.00 - 11.30	Prof. Amparo Galindo *Theoretical and computational developments for next generation thermodynamic modelling of complex fluids*
11.30 - 12.00	Dr. Nicholas Hine *Linear-Scaling Electronic Structure Calculations applied to understanding Quantum Effects in Biological Systems*
12.00 - 12.30	Prof. Sally Price *Predicting the crystal structures of pharmaceuticals – the challenges of modelling the conformational flexibility*
12.30 - 14.00	*Lunch*
14.00 - 14.30	Dr. Edina Rosta *Asymmetric activation of RAF Kinase Dimers*
14.30 - 15.30	**Keynote lecture 4: Prof. Michael Levitt** *Birth and future of multi scale modelling of macromolecules*
15.30 - 16.00	*Refreshments*
16.00 - 16.30	Dr. Julia Rice *From Quantum Chemistry to Force Fields for the Condensed Phase*
16.30 - 17.00	Prof. Michele Vendruscolo *Characterisation of Protein Dynamics using NMR Spectroscopy*
17.00 - 17.30	Dr. Ekaterina Pas *Advances and directions in computational chemistry methods for ionic liquids*
19.30 - 22.00	*Conference dinner*

Wednesday 18 March

9.00 - 10.00	**Keynote lecture 5: Prof. Gerhard Hummer** *Molecular motors and pumps in biology*
10.00 - 10.30	Prof. David Tozer *Density functionals from density scaling*
10.30 - 11.00	*Refreshments*
11.00 - 11.30	Dr. Annalaura Del Regno *Modeling the absorption of molecules through skin – a molecular dynamics study*
11.30 - 12.00	Dr. Tanja van Mourik *DNA base stacking studied with density functional theory*
12.00 - 12.30	Prof. John McGrady *In search of structure-activity relationships in molecular wires*
12.30	*Concluding comments, lunch and departure*