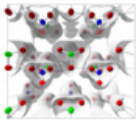
ScotCHEM Computational Chemistry Symposium



Symposium Program

- 9.30 Registration opens: the foyer, at the Gateway (University of St Andrews, North Haugh campus)
- 10.25 Opening remarks – Tanja van Mourik

Chair: Prof. Ken McKendrick, ScotCHEM Director

- 10.30 Opening of Symposium: Professor Ken McKendrick, ScotCHEM Director
- 10.45 Professor Paul Madden, FRS, University of Edinburgh:

From first-principles to the properties of ionic materials, via transferable interaction potentials

- 11.15 Dr Mark Law, University of Aberdeen:

Rotation-vibration dynamics of isomerising molecules

- 11.45 Dr Tanja van Mourik, University of St Andrews:

Methodological aspects in electronic structure calculations – examples from studies on biological molecules

- 12.15 Lunch

Chair: Dr Carole Morrison, University of Edinburgh

- 13.15 Professor John McGrady, University of Glasgow:

Extended metal atom chains: viable components for molecular electronics?

- 13.45 Dr Ruth Brenk, University of Dundee:

Assembling a screening library from scratch

- 14.15 Dr Tell Tuttle, University of Strathclyde:

The Effect of System Preparation on QM/MM Energy Profiles

- 14.45 Tea

Chair: Dr Bridgette Duncombe, University of Edinburgh

- 15.15 Professor Maciej Gutowski, Heriot-Watt University:

The challenge of on-board hydrogen storage

- 15.45 Dr Andrew Turner and Dr Herbert Früchtl, EaStCHEM Research Computing Facility:

Computational chemistry for all - the EaStCHEM Research Computing Facility

- 16.15 Closing remarks - Tanja van Mourik
- 16.20 Posters and wine

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sasol reaching new frontiers

streamline computing