

Atomic and Molecular Data Needs for Plasma Applications

Sponsored jointly by High End Computing
(HEC) Consortium, UK-AMOR and Collaborative
Computational Projects CCPQ and CCP-Plasma

13th - 15th April 2021



Engineering and
Physical Sciences
Research Council



Science and
Technology
Facilities Council

UK Collaborative
Computational Projects



Welcome!

Organisers:

- Georgia Lomas
- Martin Plummer
- Jonathan Tennyson
- Colin Roach
- Ben Dudson

Session chairs:

- Deborah O'Connell
- Martin O'Mullane

Speakers and poster presenters

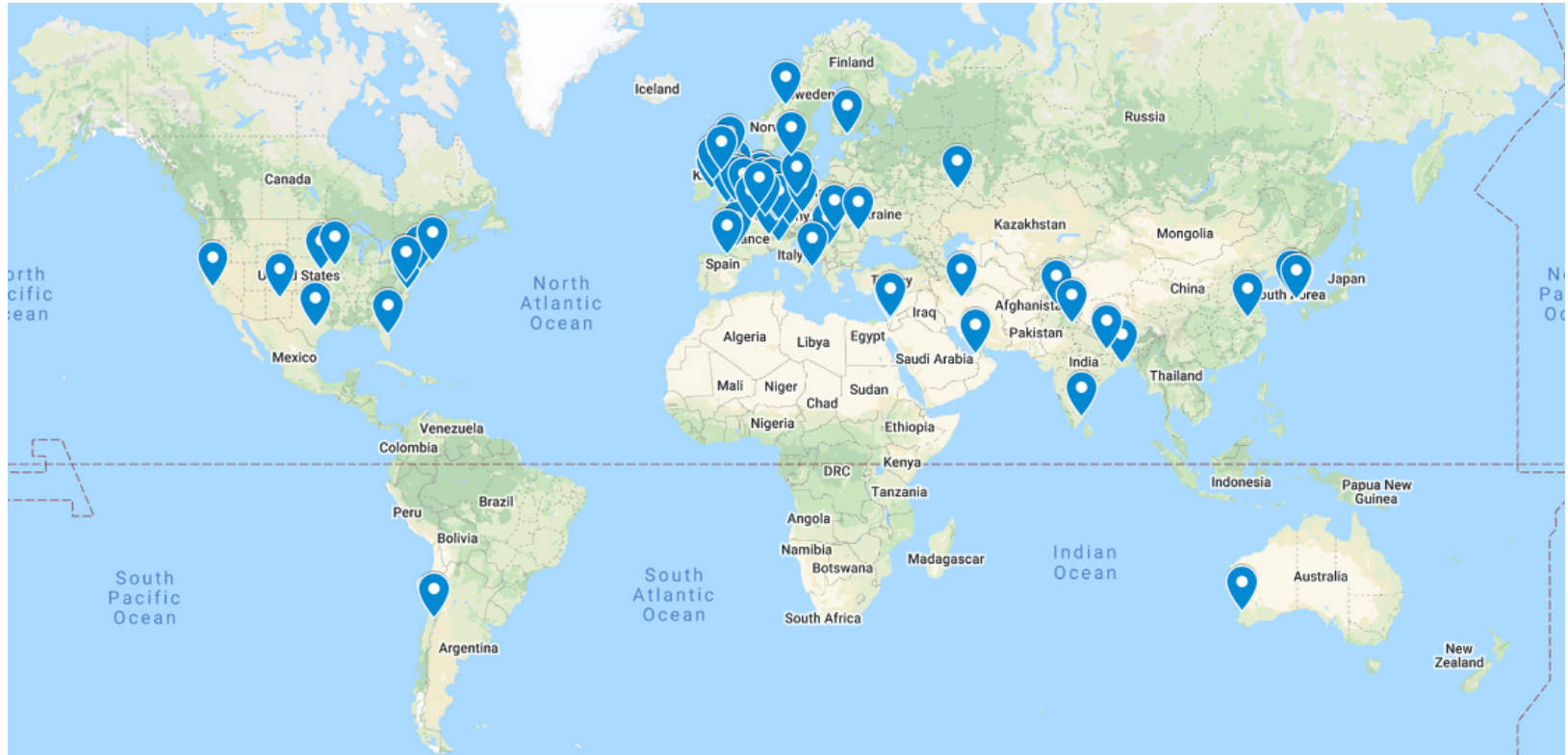


Science and
Technology
Facilities Council



Thank you!

160 people registered, >67 universities, labs and companies



Agenda

Tuesday 13th	Wednesday 14th	Thursday 15th
13:00 – 15:10 Session 1 Applications Overview Chair: Ben Dudson	10:00 – 11:00 Poster session	9:00 – 10:00 Demonstration of Quantemol tools
15:10 – 15:20 Coffee break	11:00 – 12:00 Group discussion: Fusion	10:00 – 11:00 Group discussion: Datasets
15:20 – 16:50 Spectroscopy and uncertainties for fusion Chair: Deborah O'Connell	13:00 – 15:00 Spectroscopy and uncertainties for fusion Chair: Colin Roach	11:00 – 12:00 Group discussion: LTP
16:50 – 17:10 Lightning session (poster introductions) Chair: Colin Roach	15:10 – 17:20 Atomic and molecular physics calculations Chair: Martin Plummer	13:00 – 15:00 Atomic and Molecular Applications Chair: Martin O'Mullane
	Coffee break	15:10 – 17:10 Industry and ExCalibur Chair: Jonathan Tennyson

All times UK (BST, UTC + 1)

Posters and Lightning talks

- 15 posters
- **Today:** Lightning session 16:50 – 17:10

<http://www.ccpq.ac.uk/node/24>

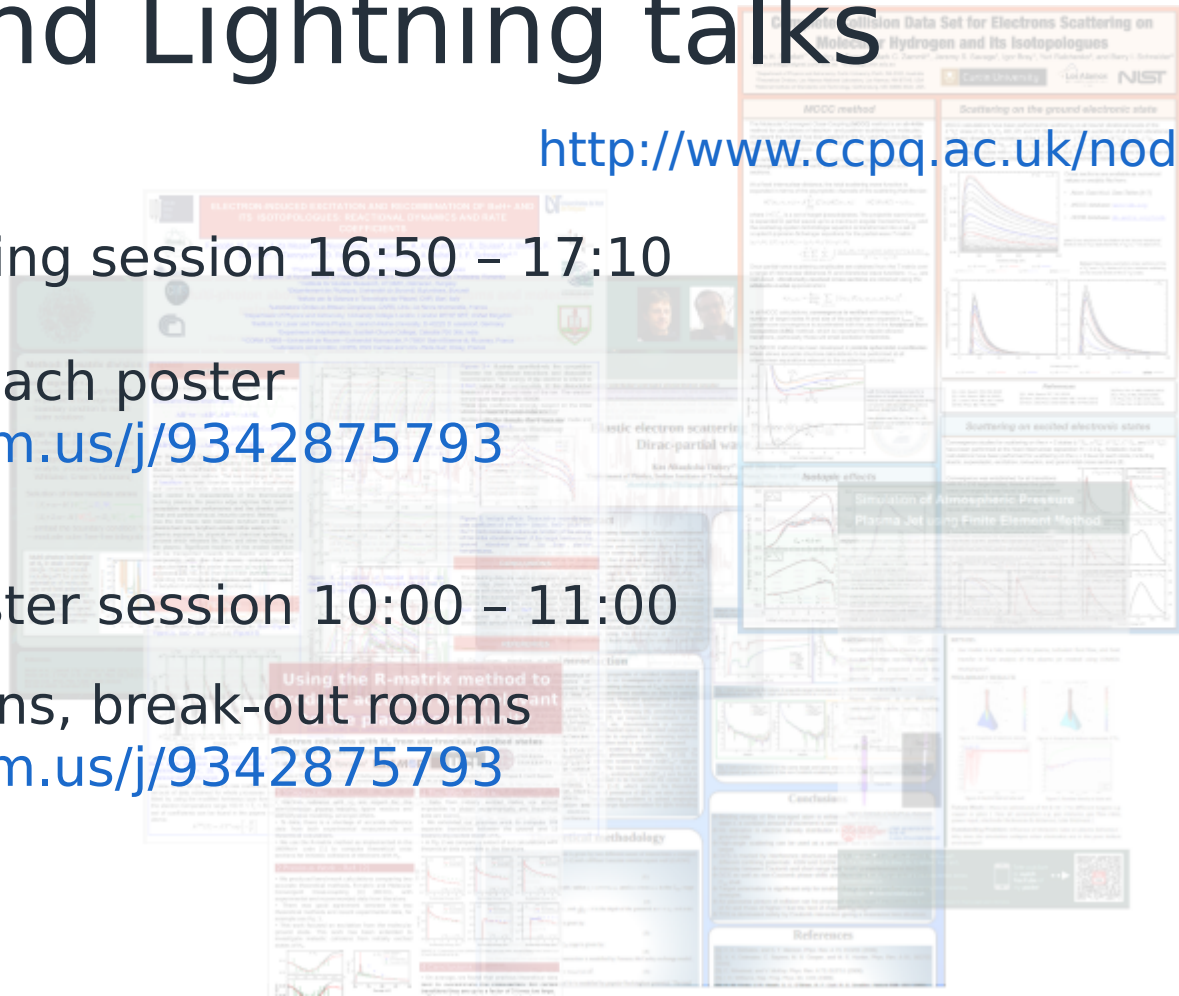
Short talks on each poster

<https://ukri.zoom.us/j/9342875793>

- **Tomorrow:** Poster session 10:00 – 11:00

Zoom discussions, break-out rooms

<https://ukri.zoom.us/j/9342875793>



Talk sessions

- **Speakers** should share their screens to present
- **Zoom** sessions will be open 30 minutes before start time
- **Talks** will be recorded unless requested otherwise (**)
- **Questions** can be asked in the Q&A tab, or by raising a hand
- **Chairs** will keep to time, allow people to unmute themselves

Today

Session 1: Applications overview

Chair: Ben Dudson

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|-------------|---|-------------|
| 13:00-13:10 | Welcome: overview by Ben Dudson (York University) | |
| | Fulvio Militello (CCFE) | 15:20-15:50 |
| 13:10-13:40 | Alternative divertor concepts and the modelling requirements/results in terms of detachment physics, power and particle loads and pumping | |
| | Andrew Gibson (Ruhr University of Bochum) | 15:50-16:20 |
| 13:40-14:10 | An overview of electron impact cross section requirements for low temperature plasma modelling | |
| | Nigel Mason (University of Kent) | 16:20-16:50 |
| 14:10-14:40 | Electron interactions with atoms, molecules, clusters and surfaces - what we know and what we need to know for next generation plasma technologies physics | |
| | Deborah OConnell (Dublin City University) | 16:50-17:10 |
| 14:40-15:10 | The importance of vibrational excitation in nitrogen plasmas | |
| 15:10-15:20 | Coffee/comfort break | |

Session 2: Spectroscopy and uncertainties for fusion

Chair: Deborah OConnell

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|--|---|--|
| | Connor Balance (Queen's University Belfast) | |
| | Interfacing atomic structure and collisional calculations with plasma diagnostics and modelling codes | |
| | Kevin Verhaegh (CCFE and York University) | |
| | Experimental investigation of the role of plasma-atom/molecule interactions on power, particle and momentum balance in tokamak power exhaust | |
| | Martin O'Mullane (CCFE and Strathclyde University) | |
| | Uncertainty estimation and integration of data into large scale modelling codes | |
| | Lightning session: brief introductions to the posters | |