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# THEORETICAL CHEMISTRY GROUP

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# COMMITTEE

**Chair: Tanja van Mourik (University of St Andrews)**  
**Secretary: Samantha Jenkins (Hunan Normal University, Changsha, China)**  
**Treasurer: Helen Chappell (University of Leeds)**

**Mark Storr (AWE)**  
**Thomas Penfold (Newcastle University)**  
**Fernanda Duarte (University of Oxford)**  
**Basile Curchod (University of Bristol)**  
**Charlotte Vale (PhD rep; University of Surrey)**

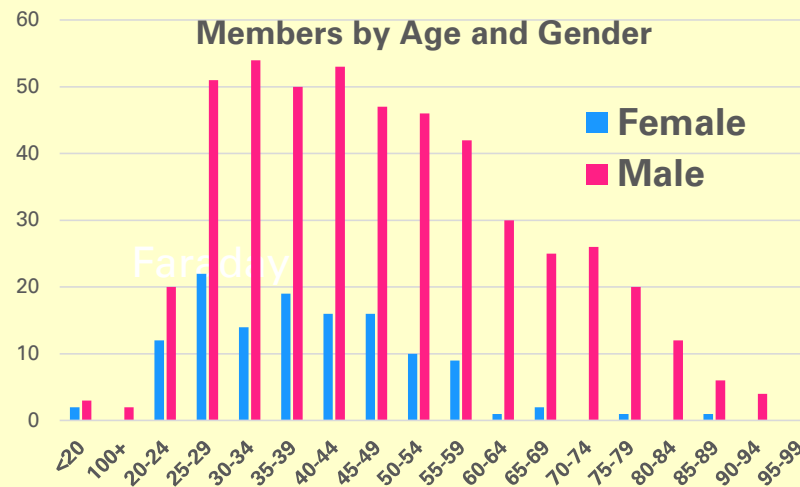
**(currently recruiting more members)**

# MEMBERSHIP

(DATA FROM NOV 2023)

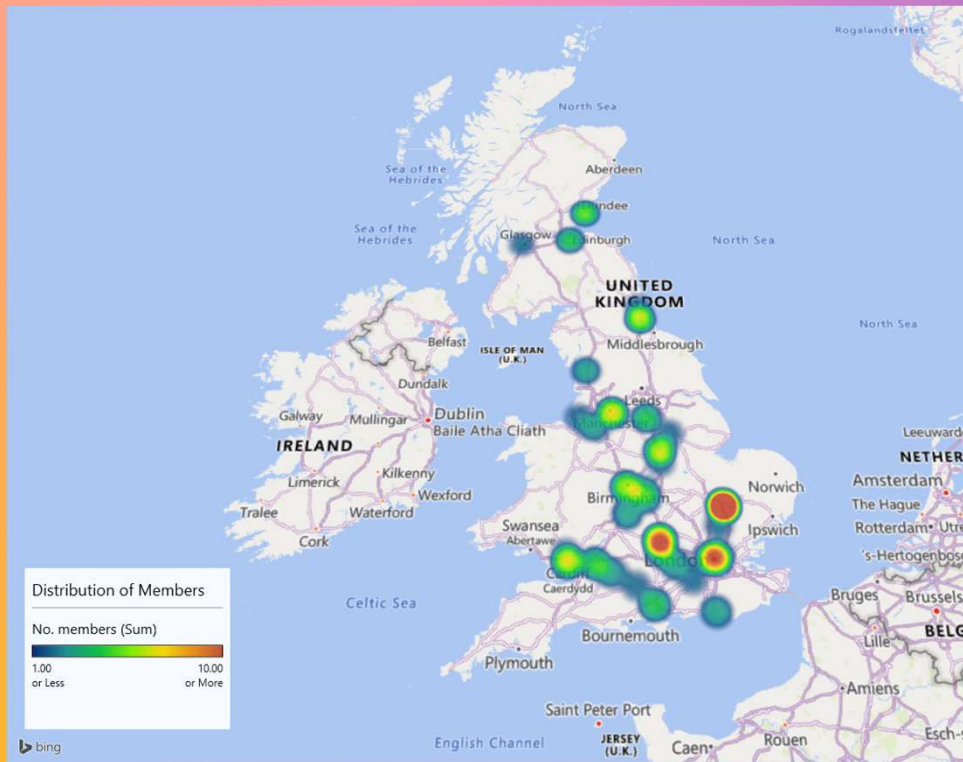
Female: 30 (20%)  
Male: 499 (77%)  
Non-binary: 3  
Unknown: 17  
Total: 649

Faraday: 23% F / 76% M

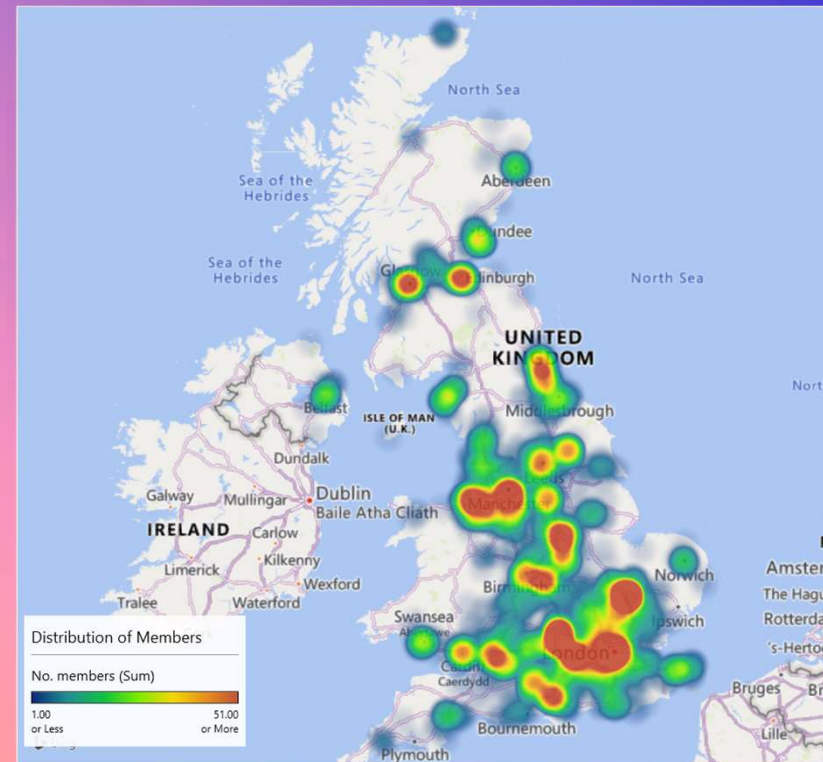


# UK distribution

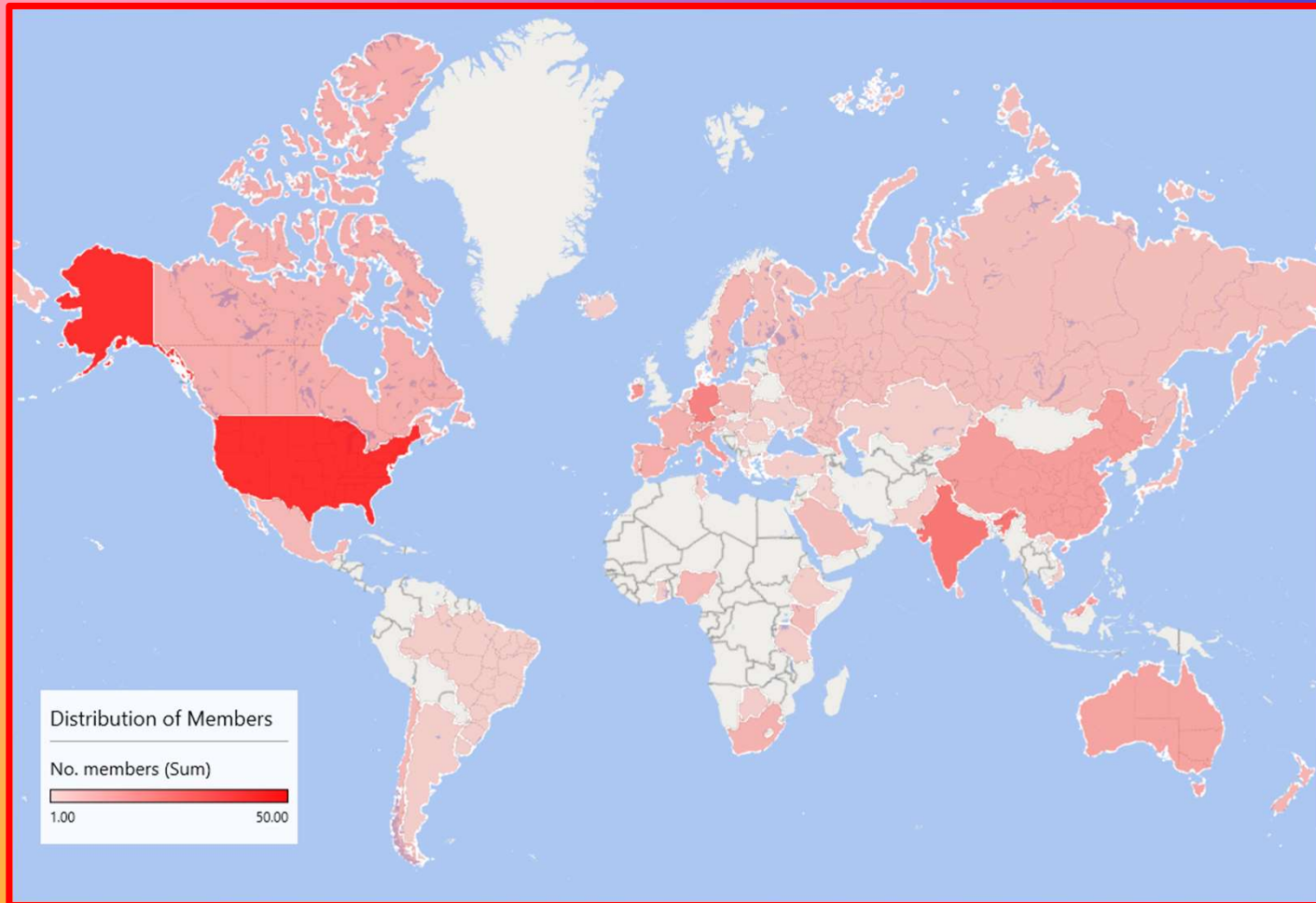
## TCG



## Faraday



# Global distribution



# Activities in 2023

## Sponsorship

**The Inaugural Lennard-Jones Centre Meeting:  
Theory and Molecular Simulation in the Physical Sciences  
Cambridge, 4th - 8th September 2023  
£700**

**Faraday Joint Interest Group Conference 2023  
3 - 5 April 2023, Sheffield  
£750**

**Scottish Computational Chemistry Symposium  
20 June 2023, Glasgow  
£500**

Activities in 2024

# Activities in 2024

## Sponsorship

**2024 ScotCHEM Computational Chemistry Symposium**  
20 June 2024, St Andrews  
£500

**Computational Molecular Science 2024**  
11-13 September 2024, Warwick  
£500

## TCG Graduate Student Meeting

**13 September 2024, University of Warwick**  
(Just after Computational Molecular Science, 11-13 September 2024)

# Graduate Student Meeting 2024

Afternoon of  
13 September 2024

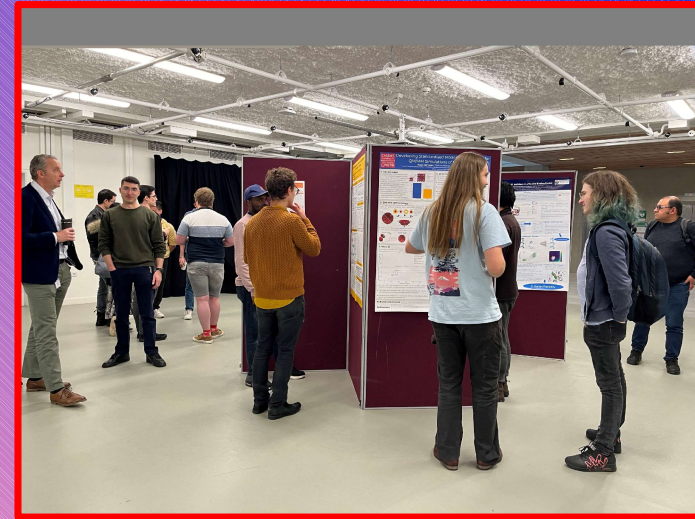
57 registrées  
22 applied for a talk  
32 posters

## Programme ¶

Agenda	Start	Finish
<b>Arrivals-/Logistics-/Introductions</b>	13:30	13:45
' <i>Tuning Zeolite Catalysts using Organic Additives</i> ' ¶ <b>Matt Robinson, University of Cardiff</b>	13:45	14:05
' <i>Excited State Dynamics of Azanaphthalenes</i> ' ¶ <b>Lauren Bertram, University of Oxford</b>	14:05	14:25
' <i>Exploring and Predicting Sigma-hole Interactions in the Cambridge Structural Database</i> ' ¶ <b>Harry Nash, University of Sheffield</b>	14:25	14:45
' <i>Transferable Insights: Predicting Molecular Crystal Structures from Prior Convex Hull Landscapes of Similar Systems</i> ' ¶ <b>Jennie Martin, University of Southampton</b>	14:45	15:05
<b>'Drinks'-/Poster Session</b>	15:05	16:00
' <i>Numerical Tensor Methods for Few Particles Quantum Systems</i> ' ¶ <b>Kammegne Brice, University of Sussex</b>	16:00	16:20
' <i>Stereochemistry of the Insertion of Diphenylacetylene in a magnesium(I) Dimer</i> ' ¶ <b>Rochelle Ferns, University of St Andrews</b>	16:20	16:40
' <i>Direct Wavepacket Dynamics for Photodissociation and Towards Explicit Solvation</i> ' ¶ <b>Leon Cigrang, University College London</b>	16:40	17:00
' <i>Spectral Map: Extracting Collective Variables for Enhanced Sampling Methods</i> ' ¶ <b>Tuğçe Gökdemir, University of Torun, Poland</b>	17:00	17:20
<b>Prizes &amp; closing remarks</b>	17:20	17:30

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**Prize for  
best poster**



**Coulson prize for  
best talk**

8 talks  
(50% F)

The infographic features three circles on a background with a color gradient from orange on the left to blue on the right. A vertical orange line is on the far left. The top-left circle is purple and contains the text '8 talks (50% F)'. The top-right circle is light purple and contains '17 registrees (24% F)'. The bottom-center circle is orange and contains '32 posters (31% F)'.

17  
registrees  
(24% F)

32 posters  
(31% F)