

Member Networks Annual Report Form

Reporting events held in 2018 and those planned for 2019

In line with the rules for member networks and to enable us to better support our networks and their activities all member networks (Local Sections, Interest Groups and Analytical Division Regions) are asked to complete this form and return it to <u>networks@rsc.org</u> or by post to: Networks Team, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF.

Deadlines

Deadline for receipt of Financial Accounts by RSC Finance Team: 8th February 2019 Deadline for receipt of Annual Report by Networks Team: 25th February 2019

If there is any reason that your committee will **not** be able to meet either or both of these deadlines please inform <u>networks@rsc.org</u> as soon as possible.

This report will be uploaded to your web page to share with the members of your network. Staff will also share a digest of all member networks activities taken solely from these annual reports with appropriate staff and governance boards and committees including Division Councils with similar interests.

Committee	Theoretical Chemistry Group
Completed by	Scott Habershon
Date	Monday, 25 February 2019

Please list below the dates of all of your planned committee meetings and, if held, AGM.

Annual General Meeting (if being held)

Date	N/A
Venue	N/A

Proposed Committee Meetings Dates

Date	Venue	
January 2020	University of Edinburgh	



2018 Events

Please report below on activities undertaken in the past year. Please select the type of event and target audience from the drop-down menus. For example, a workshop for Early Career members can be categorised as "Training/ Workshop" for "Early Career Members".

The categories are as follows:

Event Types:

- Award Lecture
- Education Event
- Networking Event
- Outreach Event
- Public Lecture
- Scientific Meeting (half-day, oneday or multi-day)
- Social Event
- Training/ Workshop
- Other

Audience:

- Academics
- Consultants
- Early Career
- Industrialists
- Members of the public
- Postgraduates & PhD students
- Retired members
- School students
- School teachers
- Technicians & Support staff
- Undergraduates

If you wish to include more detailed information about any particularly successful events or advice to share please do so in the provided space. Please append electronic copies of any meeting reports, newsletters or relevant materials to this report.

For additional events please copy and paste the table and continue as necessary.

Event Name	Biennial TCG Conference
Event Type	Scientific Meeting - Multi-day
Audience	Academics
Start Date	16 July 2018
End Date	18 July 2018
No. Attendees	50-100
Comments	The TCG conference took place from 16-18 July 2018 at the University of Sheffield. The local organizers were Grant Hill (TCG committee member) and Robert Shaw (Sheffield). The meeting was attended by approximately 70 attendees, including faculty, post-doctoral researchers and PhD students.



Keynote speakers included Marie-Pierre Gaigeot (France), Christine Mottet (France) and Paul Popelier (UK). Several PDRAs were also selected to deliver invited presentations.
The TCG conference also included an afternoon session for the annual Graduate Student Meeting. Eight final-year PhD students were selected to give presentations on their research – James Shaw (University of Birmingham) was selected as the Coulson Prize winner for best presentation.
In addition, there was a poster session, with around 20 posters presented by PhD students and PDRAs.
Conference sponsorship was kindly provided by the journal PCCP, as well as AlcesFlight.
Overall, the TCG biennial conference was a great success, in large part to the organization by Grant and Robert, as well the excellent local facilities in Sheffield.
http://grant-hill.group.shef.ac.uk/tcg2018/index.html

Event Name	ScotChem computational chemistry meeting
Event Type	Scientific Meeting - Multi-day
Audience	Academics
Start Date	14 June 2018
End Date	15 June 2018
No. Attendees	50-100
	The ScotChem computational chemistry meeting took place in June 2018, and was locally organized by Tanja van Mourik and Michael Buehl at the University of St. Andrews. The RSC TCG provided financial support for the meeting.
Comments	The first day of the meeting was dedicated to a QM/MM workshop, including hands-on sessions with ChemShell. The second day was devoted to a more traditional academic conference, with plenary speakers including Adrian Mulholland (Bristol) and Sharon Ashbrook (St. Andrews). In total 60-80 attendees were present.



Plans are already underway to repeat this event in 2019. https://www.scotchem.ac.uk/st-andrews-2018/

Event Name	Midlands computational chemistry meeting
Event Type	Scientific Meeting - One-day
Audience	Academics
Start Date	03 July 2018
End Date	03 July 2018
No. Attendees	25-50
	The Midlands computational chemistry meeting was organized by Matthew Addicoat (Nottingham Trent University) on 3 July 2018. The day featured 12 lectures given by academics, PDRAs and PhD students, as well as a poster session.
Comments	Plans are already underway to repeat this event in 2019.
	https://www.ntu.ac.uk/about-us/events/events/2018/07/midlands- computational-chemistry-meeting-2018



Awards and Bursaries

Please list any awards or bursaries presented by your committee in the past 12 months and indicate any that will be open for nomination/application in the next calendar year.

Please also include information about the application/nomination and selection processes.

Please ensure that **all** members of your network are notified of any awards or bursaries for general application. These notifications can be sent via e-alert through <u>networks@rsc.org</u>.

Award	Coulson Prize	
Award Type	Award	
Audience	Postgraduates & PhD students	
Nomination/ application deadline	N/A	
Number of nominations/ applications	8	
Award winner(s) and institution(s)	James Shaw, University of Birmingham	
Comments	The Coulson Prize is awarded annually to the final-year PhD student who is judged to have presented the best independent research presentation at our annual TCG graduate student meeting. In 2018, the prize was awarded during our biennial conference in Sheffield, held in July 2018. The winning presentation by James Shaw was entitled "Hierarchical Self-Assembly of Triblock Patchy Particles into a Tetrastack Lattice".	



Other information/comments:

Other forms of Recognition provided by your committee:



Future Activities

When planning any activities please remember to ensure that all events are logged on our events database and ensure that all contracts are sent to our Legal Team with enough time for amendments and, where necessary, approval by the Board.

Please outline any activities already in planning for the next calendar year. Please include the type of event and the target audience.

For additional events please copy and paste the table and continue as necessary.

Event Name	Graduate Student Meeting
Event Type	Scientific Meeting - Half-day
Audience	Postgraduates & PhD students
Proposed Date	June 2019
Comments	We intend to hold our annual Graduate Student Meeting again in 2019. This event is aimed at PhDs, PDRAs and other early-career researchers. Typically, around 10 final-year PhD students present their work, and the Coulson Prize is awarded to the "best" talk (as judged by the TCG committee). In addition, a poster reception is also held at this event, providing a chance for interaction between PhD students from different universities, as well as with academic staff. It is intended that this meeting will be held at the University of Nottingham, most likely in June 2019 (date TBC). Dr. Andrew Teale (Nottingham) will be taking the lead in local organization.

Event Name	Faraday Joint Interest Group Meeting	
Event Type	Scientific Meeting - Multi-day	
Audience	Academics	
Proposed Date	April 2020	



Comments	The TCG is one of the organizing committees for the next version of the Faraday Joint Interest Group meeting, provisionally to be held in Sheffield in April 2020.
Comments	We have already been involved in preparations for this event, and will continue to support the meeting by suggesting speakers and sessions, as well as providing direct financial support.



<u>Committee</u>

This information will be used to update our membership database and your web page. Please ensure that any changes to the committee are sent to <u>networks@rsc.org</u> as soon as possible.

Position	Name	Dates on committee (20xx - 20xx)
Chair	Dr. Carole Morrison (Edinburgh)	2019 - 2022
Secretary	Dr. Scott Habershon (Warwick)	2016 -
Treasurer	Dr. Scott Habershon (Warwick)	2016 -
Ordinary Members	Dr. Francesca Baletto (KCL)	2017-2020
	Dr. Abbie Trewin (Lancaster)	2018 – 2020
	Dr. Andrew Teale (Nottingham)	2018-2020
	Prof. Jochen Blumberger (UCL)	2018-2020
	Dr. Natalie Fey (Bristol)	2019-2021
	Dr. Thomas Penfold (Newcastle)	2019-2021
Chemists' Community Fund Representative (if relevant)	N/A	
Co-opted member(s) and their affiliation(s)	N/A	



Diversity & Inclusion

Please ensure this section is completed

Our trustees are aiming to embed diversity and inclusion in all of our activities and networks. Section 8 of our <u>online network handbook</u> contains more information to support our networks in achieving this and our Diversity team have <u>online Guides for Networks</u> that include actions and considerations for committees, and guides for inclusive communications and running inclusive events.

Please comment on how your group is showing that it has embraced Diversity and Inclusion within its practices. If you have diversity data from your events or activities, please include this information above.

In recent recruitment of new committee members (including chair), we have sought to ensure that fair balance in regards to gender, geography and other diversity aspects were accounted for. For example, the current committee membership is 50/50 gender-balanced.

In addition, during organization of our RSC TCG biennial conference, we also successfully sought to maintain a roughly 50/50 split in our invited **keynote** speakers. However, we acknowledge that the number of **contributed** talks presented by females was well below this target.

In our most recent committee meeting (6 February 2019), we have already discussed this imbalance and how to address it in future meetings. For example, we have already noted that we could be more proactive in directly advertising events to female academics, PhD students and PDRAs. In addition, it has been noted that simply distributing pictures of our committee membership on the RSC TCG website might encourage gender diversity in future events. With a new (female) chair in place, we anticipate that these diversity factors will be broadly improved in our future events.