

<p><b>Institution:</b> <b>Heriot-Watt University</b></p>
<p><b>Unit of Assessment:</b> <b>Sub-panel 8: Chemistry</b></p>
<p><b>1. Unit context and structure, research and impact strategy</b></p> <p><b>Strategy</b></p> <p><i>Chemistry's</i> strategy aligns with the University's 7-year <i>Shaping Tomorrow Together</i> strategy, with its focus on <i>Excelling in Research and Enterprise</i> and ambition to embed 'inspiration, collaboration, belonging and celebrating' into everything the University does. Consequently, at the forefront of <i>Chemistry's</i> academic endeavours has been to make an impact on society through our interdisciplinary approach and close collaboration with industry and business. As such, the major strategic goals for <i>Chemistry</i> since REF2014 have been to:</p> <ol style="list-style-type: none"> <li>strengthen our core activities in fundamental studies particularly in dynamics, catalysis and computational molecular modelling as exemplified by 3 new academic appointments in these areas;</li> <li>expand research activities that are interdisciplinary and bridge across traditional disciplines of chemistry, physics, biology and engineering building on strengths in the School. This is exemplified by 2 new academic appointments in this area and multiple interdisciplinary funded research projects e.g. CRITICAT, EuroPAH, GRACIOUS and PATROLS (see Section 3);</li> <li>apply existing and new fundamental research strengths into applied fields particularly those focussing on sustainability and environmental stewardship, renewable energy and the food and drink sector. This is exemplified by 6 new academics in these areas and the 153% increase in industry funded research.</li> </ol> <p>The latter goal has also provided a platform for achieving our impact strategy of providing solutions that address real world challenges and opportunities faced by industry, businesses and government bodies.</p> <p>The inclusion of applied research in <i>Chemistry's</i> strategic goals also directly align with our impact strategy goals to work with industry and business to address global grand challenges (see Horizon Proteins impact case study). These also map onto the University-wide strategy for increased research activity directly relevant to <i>Chemistry</i> in areas of sustainability, decarbonization, and healthcare. The increase in interdisciplinarity can be demonstrated by the make-up of staff in the current return from across four of the five Research Institutes within the School of Engineering and Physical Sciences (EPS). A measure of the increase in applied research can be gauged by the number of staff directly involved in collaborative activities with industry, charities and non-government agencies and government bodies, both within the UK and internationally (see Section 4).</p> <p><b>Growth and Structure</b></p> <p>As part of the EPS long-term strategy, <i>Chemistry</i> has undergone an expansion from 30 staff in REF2014, to the current return with 41 staff (39.69 FTE). This significant expansion of <i>Chemistry</i> during the REF2021 assessment period is due in part to a strategic restructuring of the internal School structures in 2016 and again in 2019 coupled with investment in recruitment and facilities</p>

## Unit-level environment template (REF5b)

by the University in this area. This strategic expansion has extended the existing subject focus so that it now includes and bridges across research in areas of mainstream chemistry, life sciences, materials science, chemical engineering, physics and food and drink sciences. To foster interdisciplinary research that addresses our strategic goals and at the same time provides appropriate support structures including sharing facilities, staff are clustered within the following research groupings (new appointments indicated in italics):

- **Molecular and Materials Chemistry** – addresses fundamental and applied atomic, molecular and materials chemistry (Adams, Arrighi, *Barker*, Bos, *Bucknall*, Costen, *Coxon*, Dalgarno, Greaves, Lee, Macgregor, Mansell, McCoustra, McIntosh, McKendrick, Nahler, Ni, M Paterson, Townsend, Vilela, Welch, Yiu)
- **Biological Chemistry** – advances in the chemical sciences to address key challenges in the life and health sciences (*Brown*, Duncan, Johnston, Leslie, L Paterson, *Melchels*, Rickman, Schweizer, Stone, Willoughby, *Yarwood*)
- **Nutritional Chemistry** – food and drink chemistry addressing production and processing. (Euston, Hill, Holmes, *Jenkins*, *Maskell*, *Pauley*, Stewart, *White*)

### Highlights Since REF2014

As a result of the implementation and achievement of the research and impact strategies, there have been some notable successes within *Chemistry* since REF2014. The highlights of which include:

- Recruitment and investment in 11 new academic staff since REF2014 - this in part has helped grow our cohort by 36.7% for this submission, with the largest increase seen in the *Biological and Nutritional Chemistry* groups (see Section 2).
- Increased the number of PhD students through both internal University - principally the HWU James Watt Scholarship scheme - and national schemes i.e. DTPs and CDTs. PhD graduations across the whole *Chemistry* unit have increased from the REF2014 figure of 9.7 to 14 per annum in this REF submission period (see Section 2).
- Significant strategic investment by EPS in *Chemistry* infrastructure and facilities of £3.41M over the REF period (see Section 3).
- Co-leadership (**Macgregor**) and participation by multiple staff (14 staff from *Chemistry*) in the EPSRC Centre for Doctoral Training (CDT) in Critical Resource Catalysis (CRITICAT) in partnership with Universities of Edinburgh and St Andrews.
- Development and leadership (**Duncan, Rickman**) of the Edinburgh Super-Resolution Imaging Consortium (**ESRIC**), a national imaging facility with a multidisciplinary approach to biological research through state-of-the-art microscopy techniques.
- Leadership of a major EPSRC Platform Grant in molecular chemical dynamics (**Costen, Greaves, McKendrick, M Paterson, Townsend** - £1.28M), which has in turn led to a recently funded HWU-led EPSRC Programme Grant to develop state-of-the-art facilities and understanding in molecular scattering dynamics (**Costen, Greaves, McKendrick, M Paterson** - £3.36M to HWU).
- Leadership roles (**Stone**) in two Horizon 2020 projects (GRACIOUS, €787K and PATROLS, €1.7M) developing classification and advanced safety assessment tools of nanomaterials.
- Co-investigator (**L Paterson**) in an interdisciplinary Programme Grant aiming to exploit laser techniques as medical therapies to address medically challenging issues (£6.13M total).

## Unit-level environment template (REF5b)

- Establishment and leadership (**Bucknall**) of the HWU led Consortium for Plastics and Sustainability (COMPASS) exploring applying fundamental research to help solve circular economy and global impact challenges associated with plastics. The collaboration began with staff from across HWU and now includes collaborators from Universities of Edinburgh, Strathclyde, Stirling, Cranfield, Sheffield and Manchester.
- Significant increase in applied research and engagement with industry, business, government and NGO since previous REF2014 particularly in the areas of materials, biomedicine and food and drink sectors. Examples of new collaborations or consultancy engagements from within the *Molecular Materials and Chemistry* group include **Bos** (e.g. Semimetrics), **Bucknall** (e.g. Zero Waste Scotland, Church and Dwight), **Mansell** (e.g. Sasol); within the *Biological Chemistry* group include **Melchels** (eg Tessengerlo Group), **Stone** (e.g. BASF, Unilever, Smart Separations, Byk), **Schweizer** (e.g. Coeliac UK) and within the *Nutritional Chemistry* group include **Euston** (e.g. Marlow Foods, Mars), **Hill** (e.g. Porth of Leith Distillery), **Holmes** (Holyrood Distillery), **Maskell** (Glenmorangie).
- Exploitation of applied research has also led to demonstratable commercial or policy changing impacts in number of areas. The most notable are: development of sustainable proteins from under-utilized by-products of food and drink industries (**Willoughby**); development of an extensive library of botanicals for gin flavouring that not only achieve desirable sensory impact, but are available for large scale production (**Hill**, Hughes, **Pauley**); informing regulatory and policy changes (i.e. changes of the directive for Carcinogens and Mutagen legislation for preventing occupational cancer (Cherrie) and changes to the regulator ECHA guidance for nanomaterials safety under REACH (**Stone**, **Johnston**). Full details given in the Impact statements.
- The Impact strategy has also helped promote entrepreneurship and innovation, which is supported by HWU's Research Engagement team, and has had direct impact through a strong track record in successful spin-out companies by members of Chemistry, e.g. Horizon Proteins Ltd (**Willoughby**), Nandi Proteins Ltd (**Campbell**), NiTech Solutions Ltd (**Ni**) and Mironid Ltd (**Adams**). Although all were founded prior to the beginning of this REF period, staff have continued to apply their research outputs to further develop the activities within these spin out companies.

## Research Governance

HWU complies with all ethical regulations for undertaking research whether performed on site or by project collaborators at other locations. Any project that includes work with live animals and human subjects requires either institutional ethical approval and/or a Home Office licence. Over the REF period **Campbell**, **Nahler**, **Leslie**, **Maskell** and **Mechels** have individually received institutional ethical approval for projects, including food and drink taste testing, blood tests to evaluate glucose and ketone levels, vaccine booster testing on cattle, and collecting and circulating tumour DNA from breast cancer and brain tumour patients. In addition, to institute ethical approval, Home Office project licences have been held by **Leslie** (to study genetically modified mice as models of cancer), **Stone** (for animal tests to assess hazards of nanomaterials) and **Johnston** (for zebra fish testing).

## 2. People

### Staffing Strategy and Development

The staffing strategy across *Chemistry* has been to maintain core strengths and capabilities and increase staff numbers in key areas. All the planned hires have been sought with expertise in interdisciplinarity across key areas and/or applied research focus. Specific target areas have been and continue to be in the medium-term planning, in areas that bridge biological chemistry and engineering and/or physics, organic chemistry with applied research activities in catalysis, and fundamental/theoretical chemistry with focus in catalysis and/or materials.

#### **Recruitment**

In this REF period we have made significant advances to achieving our 2014 objective of increasing the number of staff within *Chemistry*, despite some losses. Since the last REF submission, the following staff have left HWU: Bryce, Campbell, Cherie, John and Keane (all through planned retirement), Bebbington (moved to Montclair State University, USA), Bock (moved to the health sector in Germany), Lloyd (moved to Univ. of Lincoln) and Speers (moved to Dalhousie Univ., Canada).

Over the REF period 11 new staff have been hired who align with the staffing strategic goals. Many of the new staff come from major international laboratories in their respective fields or directly from industry, the latter to address the strategic goals of applied research. Hires into the *Molecular and Materials Chemistry* group have been: **Barker** (previously PDRA at HWU), **Bucknall** (from Georgia Institute of Technology, hired as Chair of Materials Chemistry) and **Coxon** (from Liverpool John Moores Univ.); into the *Biological Chemistry* group have been: **Brown** (previously PDRA at HWU), **Melchels** (from UMC Utrecht) and **Yarwood** (Univ. of Glasgow); and into the *Nutritional Chemistry* group have been **Holmes** (from Molson Coors Beverage Company), **Jenkins** (from Nottingham Univ.), **Maskell** (previously PDRA at HWU), **Pauley** (from Bombay Sapphire Distillery) and **White** (previously PDRA at HWU).

#### *Future Hiring*

As part of *Chemistry's* future strategy, the *Molecular and Materials Chemistry* group has an open vacancy for a chair in synthetic chemistry. It also has permission to hire up to 3 additional assistant/associate professor level staff with expertise in areas of experimental synthetic chemistry and computational chemistry with a focus on applied catalysis and/or medicinal chemistry, to help develop the strategic areas of sustainability and/or healthcare. In addition, the *Biological Chemistry* group also have permission to hire 2 additional staff in areas that bridge biological chemistry and physics and/or engineering. Five of the six positions are on hold due to Covid-19 but remain strategic goals for the immediate future.

#### **Staff Support and Development**

Each new academic received a start-up package that included dedicated modern laboratory space (either refurbished labs or new lab space totalling £624k), PhD student provision, a budget to (re)establish their research activities (totalling £461k), as well as reduced teaching loads in their first year to accelerate research activities. All new staff members have been inducted through a dedicated 'new hire' process that includes an immersive Institute specific induction process, provision of a mentor over the first 3 years in addition to University and School level training workshops, seminars and longer-term courses including the Scottish Crucible programme and Heriot-Watt Research Futures Academy. Training courses provide support for all levels of

## Unit-level environment template (REF5b)

expertise from early career researchers right through to senior academics. Courses are open to all University staff.

Research activity across the University is regularly monitored with an annual Performance and Development Review (PDR). The PDR, completed by all staff, reviews the previous period's performance and includes a forward job plan that both ensures personal research targets, as well as career development and training opportunities, are being met. It also provides a mechanism to support research activities and increase skills both directly and indirectly related to the research activities, including external funding, publications, researcher supervision and impact. The PDR also allows strategic decisions to be taken by the Institute level and School level heads to maximise research opportunities and collaborations whilst balancing administrative and teaching loads for individuals.

Over the REF period, personal and professional development activities, resources, opportunities and achievements offered through the Research Futures Academy have been widely used by the Chemistry staff. Staff within Chemistry have all attended the required training courses including those related to ethics and PhD/PDRA supervision, which reflects the importance the University places on ethics and diversity (see below) as well as PGR supervision. However, all staff have attended more than the minimum required courses, including staff mentoring, time management, impact through public engagement, leading resilient teams, and mental health awareness training for managers, among many others. In addition to these short, focussed training and development courses, 3 staff (**Melchels**: 2016, **Mansell**: 2014, **Nahler**: 2014) from *Chemistry* have attended the annual intensive six-day Scottish Crucible training programme aimed to help researchers think differently, inspire them, and discover skills and attitudes likely to make their research more innovative. Direct outputs of this programme have been the development of a schools-level project based around 3D printing, a new collaborative research project exploring novel Ni catalysts for polymerisation, and a personal Fellowship application to EPSRC.

In addition, funding for career development including pump-priming research collaborations, supporting conference travel, development of new research directions, and research opportunities has been competitively won from the Scottish Funding Council through Research Pools; ScotChem (Chemistry), SUPA (Physics) and SULSA (Life Sciences). The Pools' Postgraduate and Early Career Researcher Exchanges (PECRE) funds have been used by several early career staff (**MacIntosh**, **Mansell**, **Vilela**) as well as 7 research fellows from various research groups for extended research exchanges to 14 international research labs in USA, Canada, Netherlands, Switzerland, Portugal, Germany, France and Hong Kong. All have resulted in at least one joint paper in leading journals incl. *J. Am. Chem. Soc.* and *Nature Chem.* In addition, **Bucknall** and **Vilela** have benefitted from Pools Engagement in European Research (PEER) funds to aid an EU funding proposal application.

The staff PDR process also forms the basis for initiating internal promotions, which during the REF period includes:

- Promoted to Professor: **Costen** (2016), **Euston** (2017), **Leslie** (2017) and **Townsend** (2020)
- Promoted to Associate Professor (Reader): **Bos** (2016), **Kraft** (2018), **Melchels** (2018), **Maskell** (2019) and **Townsend** (2013).

Members of *Chemistry* make a strong contribution to the running of the University by holding key leadership and strategic roles:

## Unit-level environment template (REF5b)

- **M Paterson** is the current Head of Institute of Chemical Sciences (ICS), previously held by **McKendrick** and **Macgregor**.
- **Stone** is current head of Institute of Biological Chemistry, Biophysics and Bioengineering (IBBB), sits on the HWU Strategy Implementation Group and serves as an elected member of the HWU Senate (currently serving second term), previously held by **Duncan**.
- **Maskell** is Director of the International Centre for Brewing and Distilling (ICBD).
- **Leslie** is Director of Research for EPS, a role previously held by **Macgregor**.
- **M Paterson, Stone** and **Leslie** sit on the EPS Senior Management Group, positions previously held by **McKendrick, Duncan** and **Macgregor**.
- **Duncan** was Senior Academic Lead for Strategy for Heriot-Watt University and sat on the Pan-University Strategy Steering and Implementation group prior to secondment to the UKRI.

## PGR Students

*Chemistry* attracts postgraduate researchers, postdoctoral research associates and eminent researchers from across the world. A total of 98 PhD students who were supervised by *Chemistry* staff have completed and submitted their thesis during the REF period with an average completion rate of 14 per year. The total number of PhD students who graduated during the current REF period has increased by 102% with the average number graduating per year increasing by 44% (cf. REF2014). These students have been funded via the CRITICAT CDT, standard EPSRC DTP studentships, HWU's fully funded *James-Watt Scholarship* (JWS) scheme, CASE studentships (i.e. AstraZeneca and GSK), European Commission (FP7) funding and direct sponsorship from industry (i.e. Byk).

HWU is a founder member of the EPSRC CDT in Critical Resource Catalysis (CRITICAT) run jointly with the Universities of Edinburgh and St. Andrews. Students undertake an initial 6-month training period to develop key scientific and transferable skills followed by a 42-month PhD research project. The first of five annual PhD cohorts started in September 2014 and 17 students have started their PhDs under supervision with *Chemistry* at HWU. CRITICAT has fostered collaborative projects between the three participating institutions, as well as joint projects between chemistry and engineering at HWU e.g. Andresen (UoA12)/**Mansell, McIntosh/Garcia** (UoA12), and **Yiu/McCoustra**. The further sustainability of CRITICAT is seen in the EaSI-CAT initiative (from Sept 2019) in which industry funding provides an additional 6 months stipend to facilitate industrial placements and industry-led group projects.

## Equality and Diversity

Focused action plans overseen by senior staff ensures the University's equality and diversity activities go beyond our legal requirements and Athena Swan commitments, ensuring that everyone from across the University community understands how they contribute to a culture of 'Inclusion for All'. This requires all staff, researchers and PhD students in *Chemistry* to complete the basic equality and diversity awareness training. Staff also have the option to extend the training with other workshops that include diversity in the workplace, diversity in learning and teaching and equality analysis, unconscious bias, equality essentials, equality impact assessment and cultural awareness training, all of which are offered through the University's Research Futures Academy. An example of the effect this is having on gender balance is indicated by the number and variety of roles undertaken by women in *Chemistry*, including leadership roles (**Stone** and **Maskell** – see

## Unit-level environment template (REF5b)

above), Institute UG Discipline Heads in Chemistry and Biology (Howarth and **Maskell**, respectively – previously held by **Arrighi** and **Johnston**, respectively), Director of Nanosafety Research Group (**Johnston**) and IBBB Seminar series lead (**L Paterson**). In addition, PDRA representatives on School safety committee and elected Chairs of Postgraduate Societies (for ICS and IBBB) are currently all women. The latter Societies are student-led and control their own budget (from respective Institutes) to support professional and social events they organise, including seminars from guest speakers, outreach events such as schools and public science festivals, and activities to help foster networking.

In 2020, Heriot-Watt made a successful submission to renew our Athena Swan Bronze Charter Award; this has been conferred until 2026 reinforcing our ambition to put EDI at the heart of our future strategy. In addition to Heriot-Watt University award, a successful EPS Bronze application (awarded 2015 and renewed 2020) was led by the school-wide Self-Assessment Team (SAT) that included several *Chemistry* members (**Campbell, Duncan, Johnston, Mansell, McIntosh** and **Melchels**). The award led to a significant investment in Early Career Researcher (ECR) career development including a new mentoring scheme, specifically for PDRAs pairing mentees with experienced academics. In a notable example of this within the *Molecular and Materials Chemistry* grouping, Haddow was awarded a Daphne-Jackson fellowship (2018-20) and was mentored by Macgregor. Commitments under Athena SWAN related to work/life balances has also allowed Stone to work on a 0.8 FTE appointment whilst remaining a Head of Research Institute and **Bos**, Lloyd (before leaving HWU), **Greaves, McIntosh, M Paterson** and **Rickman** to take paternity leave during the REF period.

To help improve gender balance and diversity, adverts for new hires require a statement encouraging women and minorities to apply and candidates who have a disability and/or have served in the Armed Forces must be interviewed if minimum selection criteria are met. A gender balanced interview panel who have all undertaken unconscious bias training is also mandatory. Our recruitment over the REF period (including **White** and **Maskell**) has brought the overall percentage of female staff in *Chemistry* to 21% (cf. 10% in REF2014), with 42% of hires of PDRAs being women. The percentage of female PhD students for each academic year has varied between 40 and 45%, which is above the national average for Chemistry. The gender balance figures for PDRA and PhD students is very encouraging, and the future recruitment strategy for *Chemistry* staff will prioritise improving the gender balance.

### 3. Income, infrastructure and facilities

#### Income

Total HESA research income for *Chemistry* during this assessment period has increased overall by 52% (not including Research Councils income-in-kind) compared to REF2014. Although modest increases in income have been obtained from UK-based research funding agencies (21%), much more significant increases have been made in funding from UK-based charitable sources (105%), EU sources (132%) and UK and non-EU industry (153%). The increase in industrial funding clearly demonstrates the success in achieving *Chemistry's* strategy to expand applied research. Additionally, an increase of 139% of in-kind income from UKRI Research Councils have been received by **Arrighi, Bucknall, Bos, Euston, Greaves, Macgregor, McCoustra** and **Vilela** for use of the National facilities, including ISIS Neutron facilities, Diamond Light Source as well as ARCHER and CIRRUS Supercomputers. Use of these facilities exploiting neutron diffraction, small angle scattering, quasi- and inelastic scattering and reflectivity, as well

## Unit-level environment template (REF5b)

as XANES, has been critical to the increased research activities in areas including alternative energy, catalysis, polymer composites and rubber recycling.

**Notable Funded Projects***Molecular and Materials Chemistry*

- Based on earlier EPSRC (**Costen, Greaves** and **McKendrick**, £808k) and Leverhulme Trust (**M Paterson**, £142k) funding and other joint grants in the previous REF period, led to the award in 2016 of the EPSRC Platform grant (*'Dynamical Chemical Processes'*, **Costen, Greaves, McKendrick, M Paterson, Townsend**, £1.28M). This has enabled high risk proof-of-concept studies in both experiment and theory, supported 7 different PDRAs, and resulted in >35 peer reviewed publications, including 3 in *Angew. Chem. Int. Ed.* and 2 in *Nature Chemistry*. It has also resulted in additional funding from standard mode EPSRC grants: novel non-linear optical fibre sources for ultrafast time-resolved molecular dynamics (**M Paterson, Townsend** and Travers (HWU, UoA 9) (£589k)), novel use of reactive scattering at ionic liquid surfaces (**Costen, McKendrick**, Bruce and Slattery (York), Minton (MSU, USA) and Wasserscheid (Friedrich-Alexander University, Germany) (£680k)) and also both EPSRC (£520k) and Leverhulme Trust (£192k) funded projects to develop new electronic structure and quantum dynamical methodologies for modelling photodynamical processes (**M Paterson**, Kirrander (Edinburgh)) as part of a new Quantum Molecular Dynamics Edinburgh research consortium.
- Building on the strengths supported by the Platform grant, **Costen, Greaves, McKendrick** and **M Paterson** have started (June 2020) an EPSRC Programme grant (*'New Directions in Molecular Scattering'*, £3.36M to HWU) with the University of Oxford. This project will extend state-of-the-art experiment and theory to challenging and previously intractable problems relevant to the atmospheric, combustion and plasma science. The project will fund 12 individual PDRAs and through leveraging postgraduate funding ca. 15 PhD students will be trained, in addition to ca. 20 final year Masters project students.
- Co-directed by **Macgregor**, members of the *Molecular and Materials Chemistry* group (**Barker, Bos, Bucknall, Dalgarno, Lee, Mansell, McCoustra, McIntosh, Ni, M Paterson, Vilela, Welch, Yu**) have collectively been involved in the EPSRC CDT in Critical Resource Catalysis (CRICAT) (£4.33M from EPSRC, matched by the partner universities (HWU, St Andrews, Edinburgh) and with £300k direct support from Industry (AstraZeneca, Syngenta and Sasol).
- **Macgregor** has attracted £1.03M for computational modelling in collaboration with Weller (Oxford/York, as part of the latter's £1.9M EPSRC fellowship exploring metal-sigma-interactions) and with Whittlesey (Bath) on heterobimetallic chemistry. These projects have resulted in 28 papers (incl. 8 in *J. Am. Chem. Soc.* and 5 in *Angew. Chem. Int. Ed.*).
- **Bucknall** has secured over £1.2 M of funding from a range of UK-based multinational industries (including Iron Ocean, Weir, TechnipFMC, MacTaggart Scott and Recircle) in various areas of applied research. An example of the applied research for Iron Ocean (£214k) has been the development of a prototype offshore survival garment to prevent death from cold water immersion. This garment won both the SPE Offshore Achievement Award for HSE Innovation in 2019 as well as the Corporate Vision Oil and Gas Award for Best Specialist Protective Clothing Manufacturer in 2020.
- **McCoustra** and **M Paterson** are part of the Horizon 2020 funded European Training Network EuroPAH (HWU portion - £317k), coordinated by Aarhus University (Denmark) with



## Unit-level environment template (REF5b)

Universities of Leiden, Paul Sabatier (Toulouse), Westfälische Wilhelms (Münster), Cologne, Radboud (Nijmegen), Milan, Liverpool and Bristol plus a number of non-academic partners including Graphic Science Ltd. The scientific focus of EuroPAH is to understand the role and impact of polycyclic aromatic hydrocarbons (PAHs) in the universe.

- **McCoustra** is part of a multinational team (IceAge) awarded 31 hours of observational time under the Director's Discretionary Early Release scheme on the James Webb Space Telescope (JWST) to explore chemical evolution of ices during star formation.
- **McIntosh** was awarded a New Investigator award from EPSRC (£307k, 2019) looking into using discrete polymetallic complexes as soluble models of heterogeneous catalysts. The grant funded a 2-year PDRA, with a DTP-funded PhD student working on a related project. To date the work has resulted in conference presentation at RSC Coordination and Organometallic Chemistry Discussion Group, (Dublin, Dec 2019) and a paper in *Chem. Eur. J.* (2020).
- Support from ScotChem research pool has provided travel and subsistence for early career staff development and EU-wide proposal development through PECRE and PEER funding (£41.2k), respectively. One notable success from PECRE funds resulted from the study visit by Purcell (PDRA) to Minton at Montana State University in 2014. The subsequent on-going collaboration with **Costen** and **McKendrick** has led so far to 8 papers incl. in *J. Phys. Chem. C* and *Langmuir*, and has also directly contributed to 2 recently awarded EPSRC grants (totalling £6.56M) including a Programme Grant. Another notable success was the visits to Hong Kong University by Tobin (PDRA) and **Vilela** resulting in 8 papers incl. in *J. Mater. Chem. A* and *Chem. Soc. Rev.* and a recent joint grant application.

*Biological Chemistry*

- **Stone** is involved in 3 four-year Horizon 2020 projects (a) GRACIOUS (**Stone** is coordinator, €787K) is developing a highly innovative science-based Framework to enable practical application of grouping, leading to read-across and classification of nanomaterials and nanoforms, (b) PATROLS (€1.7M) will deliver advanced and realistic tools and methods for nanomaterial safety assessment, and (c) BIORIMA (€242k) which is developing a risk management framework for medical applications of nanomaterials.
- **Duncan** and **Rickman** were part of the co-investigator team on a €2.5M ERC award. This award was focussed on the development of novel TCSPC SPAD arrays and their application in the study of the biochemical organisation and interactions of proteins in cellular systems. This project was delivered by an interdisciplinary team comprising electrical engineers, microchip designers, optical physicists and cell and biochemical researchers (PI Robert Hamilton, University of Edinburgh), with €1.1M spend in Heriot-Watt between 2014-19.
- **Duncan** was Coordinator of the EU-funded CATAcURE project (€1.1M, 2016-19) and was part of the £9.8M EPSRC Inter-Disciplinary Research Centre 'Proteus'; both projects developed non-invasive photonic theranostics – a personalised approach to cancer combining therapy and diagnostics.
- **Melchels** was awarded a New Investigator grant from BBSRC in 2019 (£563K) for 'SAVE: Single-Administration Vaccine Enhancement' to develop novel burst-release scaffolds for vaccine delivery. Melchels has also received an additional total of £335k from EPSRC, Melville trust, Medical Research Scotland and Royal Society to develop 3D printing for biopolymers and *in vitro* models for pancreatic cancer and brain tumours.

## Unit-level environment template (REF5b)

- **Rickman** received funding from the Wellcome Trust in 2019 (£500k HWU portion). This award is focussed on the investigation of the Type VI secretion system and its role in bacterial pathogenicity of fungal cells. The findings from this project will have applications in treating human fungal infections and antimicrobial resistance. This project is an international collaboration with Universities of Dundee, Edinburgh, Newcastle, Exeter and Berlin.

*Nutritional Chemistry*

- **Euston** is project coordinator of the Horizon 2020 project MARISURF (€1.2M to HWU) between 5 universities and 8 companies in 5 European countries to discover, isolate and scale up fermentation of microbial biosurfactants and bioemulsifiers.
- **Euston** has had 2 KTP projects, one with Macphie of Glenbervie (£158,257) that explored the use of serpin barley protein Z extracted from whisky pot ale as an egg replacer in baked goods; and the second with Nandi Proteins (£109,010) developed a fluorescence based on line sensor coupled with an agent-based Bayesian logic model to allow prediction of processing conditions to obtain proteins with required functionality.
- **Euston, Campbell & Stewart** have secured over £1.06M from a BBSRC funded project and Innovate UK for industry focused projects on related projects that explored formation of oleogels in triglyceride oils as replacements for saturated fats, as well as those derived from food processing waste streams including from sausage casing manufacturing and also rapeseed oil press cake.
- **Euston** has used 500k core hours on CIRRUS and has been awarded 21600 kAU on Archer through the HECBIOSIM EPSRC project, to support both the MARISURF (modelling surface behaviour of glycolipid biosurfactants) and BBSRC (modelling oleogel formation) projects.
- **Hill** has secured £380.2k through combined direct industry support and Innovation and Interface Food and Drink vouchers for product development (e.g. Isle of Harris Distillery, Borders Distillery, Tipplebox, Verdant Spirits and Highland Vodka) and feasibility studies (e.g. Scottish Botanicals, Red Squirrel Brands) as well as longer term studies for The Three Stills Ltd and Nikka Distilling Company.
- **Hill** and **Maskell** have secured a KTP project (£152k) with Muckle Brig Ltd to identify new yeast strains and develop and embed optimal propagation, fermentation and sensory analysis methods suitable to produce unique whisky.
- **Maskell** has secured a KTP project (£158k) with St Andrews Brewing Company to develop and apply quality systems in a small-scale brewery for production and innovation.

**Infrastructure and Facilities**

HWU have invested heavily in shared facilities and development of infrastructure within the chemistry assessment unit, with a total of £3.41M internal investment with additional external funding supporting equipment purchases. The equipment is critical to underpin the research across *Chemistry*.

***New Infrastructure and Upgrades****Molecular and Materials Chemistry*

- *Single Crystal (SCXRD) and Powder X-ray Diffraction (PXRD) equipment*: The aging SCXRD was replaced for a state-of-the-art dual X-ray source (Cu and Mo) system (Bruker D8 Venture) which is the first of its kind to be installed in the UK (HWU contribution £108.7k, 2019). The new SCXRD has provided greater support of industry activities with a contract

## Unit-level environment template (REF5b)

with Cambrex Corporation to supply their molecular structural analysis needs. The PXRD system (Bruker D8 Advance) has been updated via £95.5k funding from the University to maintain its capability with new X-ray tube, generator and water chiller. In addition, £305k EPSRC funding has been awarded for purchasing a Malvern-Panalytical Empyrean instrument to complement our PXRD capabilities and develop new areas of research in strategic areas.

- *Liquid chromatograph mass spectrometer* facility: Shimadzu (Nexera LC-2040C 3D UHPLC with LCMS-2020 mass detector) (£134.6k, EPSRC Equipment grant). Integrated analytical Ultra High-Performance Liquid Chromatography (uHPLC) Instrument with Dual Ionisation Single Quadrupole Mass Spectrometry Detector (MS). Sciex API 3000 Triple Quadrupole MS system with HPLC front-end (provided by Charles Rivers Lab). This equipment significantly expands the research capabilities of Chemistry and will promote research in strategically important fields, particularly in healthcare.
- *Peptide Synthesis Facility* (~£80k via Coxon start-up): Facility consists of a CEM Liberty Blue microwave-assisted automated single channel peptide synthesiser, Teledyne EZ Prep preparative HPLC, Agilent 1100 series analytical HPLC with autosampler and variable wavelength detector, Labryo freeze drier and heated shaking platforms for manual peptide chemistry production on a 1 – 1000 mg scale. This will interface with the mass spec. facility for peptide identification and characterisation activities. This facility will be able to provide designed peptides for research purposes to colleagues within HWU as well as providing a route to external activities.
- *Upgrade to NMR facilities*: Acquisition of a HRMAS probe (£12.6k, 2014) expanded the capability to work with the full range of materials from powdered solids to mobile liquids making the system unique in Scotland. A 'SampleCase' autosampler (£21.5k, 2016) has been added to increase sample throughput and update to a more robust instrumentation platform. Update to a AVIIIHD console (£162k (2018)) and installation of advanced software (TopSpin 3.6) enables a greater range of experiments, rapid 2D acquisition through NUS (non-uniform sampling), superior quality of data from new sequences (e.g PureShift, multiple solvent suppression) and better temperature regulation.
- *Scottish High-Field NMR Centre (SFC)*: A successful EPSRC award (£1.5M) enabled an upgrade of 800MHz spectrometer to be housed at the University of Edinburgh to which HWU researchers have open access. Additional investment from ScotCHEM and SULSA (£86k) has funded NMR-scientific meetings, a postgraduate NMR training workshop and facilitated collaborative use of NMR by Scottish scientists.
- *Benchtop NMRs*: A Nanalysis NMReady 60 Spectrometer (£30.5k, 2018) and an Oxford Instruments X-Pulse Multinuclear NMR Spectrometer (£73.2k, 2020) benchtop research NMRs have been purchased. Their portability provides options for in-situ studies such as frequently being incorporated into flow reactors/systems for in-line monitoring by NMR.

*Biological Chemistry*

- The FlexBio open-access pilot scale bioprocessing facility opened in 2015 with funding from the Industrial Bioprocessing Innovation Centre (IBioIC - £1.13M) and HWU internal support (£1.01M). The facility provides scale-up facilities of 15 - 100 litres combined with a highly flexible, integrated approach to total process development on a single site.
- The University has invested significantly in Biological Chemistry in the current REF period; £0.7M was spent on refurbishing laboratories in 2014/15 to provide an entire floor of state-

## Unit-level environment template (REF5b)

of-the-art tissue culture and laboratory space specifically for new staff all based within Chemistry.

- Vitrocell dry powder cloud generator (funded by PISC (Peta International Science Consortium) for equipment (Brown, £90k)) for exposing 3D lung cell cultures to aerosols for evaluating inhalation toxicology.

#### *Nutritional Chemistry*

- Upgrade to distillery and to brewery facilities including two dual purpose fermentation vessels (~£250k), as well as upgrade to control system and boiler (~£18k) for brewery, installation of spirit safe, extraction system for distillery and installation of new vacuum still (total ~£27.5k)

#### **Existing Facilities**

In addition to individual research group equipment and those detailed in 'New infrastructure and Upgrades' above, Chemistry staff have access to a wide range of open-access shared user facilities. These facilities are managed by dedicated technical staff and overseen by Chemistry management groups. The most significant of these facilities include:

#### *Molecular and Materials Chemistry*

- *Solution and solid-state NMR facilities:* Bruker AVIII400 Spectrometer with BB(F)O probe, Bruker AVIII400 Spectrometer with BB(F)O and solid-state CPMAS and HRMAS probes, Bruker AVIIHD Spectrometer with BB(F)O probe.
- A suite of IR equipment including two Nicolet iS5 FTIR spectrometers and a PerkinElmer Spectrum 100 FTIR spectrometer
- *Solvent purification system:* MBRAUN SPS5 system providing 5 high purity common solvents (THF, toluene, DCM petroleum ether, acetonitrile) in high volumes.
- *Elemental Analyzer:* EAI CE440 Elemental Analyzer of C, H, N and S of all organic compounds.

#### *Biological Chemistry*

- *Edinburgh Super-Resolution Imaging Consortium (ESRIC):* A HWU-Univ. of Edinburgh joint open-access facility for advanced super-resolution microscopes. Located at HWU are an Olympus IX81 Motorised TIRF microscope for single molecule localisation microscopy (PALM, dSTORM), a Leica SP5 SMD scanning confocal microscope for TCSPC FLIM and FCS and a Leica SP8 3X dual STED microscope for stimulated emission depletion microscopy. The facility includes dedicated advanced analysis software and data storage and is operated by a full-time manager. Although started in the previous REF period, additional funding from the Wellcome Trust (PI **Duncan**, £778K, 2018-23) has helped extend its activities. The ESRIC was recognised as the **Times Higher STEM Research Project of the Year 2018**.
- *Tissue Culture Facility:* A core facility for internal and external users to provide equipment and expertise for the culturing of mammalian cells and human materials up to containment level 2 and GM Class 2 This facility has a part time manager.
- *Wet Laboratory Facility:* A core facility for internal users to provide large equipment for research laboratories. All equipment is fully serviced and includes water systems, autoclave capabilities, prokaryotic culturing, centrifugation and cryogenic storage. This facility has a part time manager.

## Unit-level environment template (REF5b)

*Nutritional Chemistry*

- A 2-hectolitre experimental plant for beer or spirit production includes a mash tun, cereal cooker, lauter tun/infusion mash tun, and a mash filter. These feed in to three brewing vessels which can be used for the production of ale or lager wort, and malt or grain distillers' wash, from a variety of raw materials. Green beer produced can be cask matured, and there are also facilities for filtration together with a bright beer tank and equipment for bottling.
- A *pilot distillery* consisting of a 25-litre wash still and an 18-litre spirit still with two alternative neck designs, a nine-plate bubble cap column and a water-cooled condenser column.
- *Micromaltings* for production of less than 200-litre brew-length, including maltings, mash-baths, and milling machines.
- A dedicated analytical laboratory for testing products from brewing and distilling processes that includes HPLC-UV/RID/RF; HS-GC-FID/ECD and SPME-GC-MS and can perform analysis for higher alcohols, vicinal diketones, carbohydrates, phenols, esters, cask extracts, and hop and gin volatiles.
- Facilities aimed primarily at supporting food and drink research includes a Zwick Roell texture analyser, Kibron Ezi-Pi surface tensiometer for measuring interfacial and surface tension, Malvern Mastersizer MS200 laser diffraction particle sizer, AktaPurifier (chromatographic separation (IEX, HIC, RP, SEC) of proteins, polysaccharides and nucleic acids), two stage valve high pressure homogenizer (APV), Thermo Fisher dual beam scanning UV/VIS spectrophotometer, Lyotrap small freeze drier, Edwards Super Modulyo large scale freeze drier, IKA RV 10 auto pro V rotary evaporator and a Leica TCS2 confocal and a number of various Zeiss optical microscopes.

**Shared Facilities**

Additional shared facilities are available to all researchers within HWU, those used by *Chemistry* in the REF period include:

- Avery Denison 500kN (static) and 3000kN (compression) testing rigs, Instron 100kN (static) and 500kN (dynamic) uniaxial testers.
- Environmental scanning electron microscope (ESEM), FEI Quanta 3D FEG ion beam microscope and Atomic Force Microscope (AFM)
- Malvern Kinexus controlled stress/strain rheometer, with cone and plate and cylinder accessories, and a bicone and Du-Nuoy ring for interfacial rheology.

**University Underpinning Support**

In terms of research support for academics the university has a centralised research and business development professional support team, the Research Engagement Directorate (RED). Although centralised, this unit works directly with individual researchers and strategies for UoAs. The individual teams in RED are listed below with examples of how they have worked with *Chemistry* researchers:

- *Research Development* - provides specialist support for academic staff seeking to win research funding. Facilitating all funding activity including e.g. running mock panels for successful major bids (e.g. **McKendrick's** EPSRC Programme Grant, 'New Directions in Molecular Scattering' in 2020).

## Unit-level environment template (REF5b)

- *Business Development* – works with academics to increase research income from industry and business (e.g. facilitating KTP submissions such as Recyclatech Limited and MacTaggart Scott with **Bucknall**).
- *Research Grants Office* – assists academics with their post-award management of their externally funded research grants and contracts.
- *Policy, Strategy & Impact* – ensuring and supporting research policies. The unit supports approaches to impact and includes the award-winning Public Engagement Team (e.g. facilitating activities at science festivals such as **Duncan**, 'Science, Jellyfish, Science & Art', Edinburgh International Science Festival 2016).
- *Legal Services* – provides essential advice on contract and IP arrangement (e.g. provided effective support for establishing contractual relationships with **Adams** and Mironid, assisting substantial contract renewal in 2020).

#### 4. Collaboration and contribution to the research base, economy and society

*Chemistry* staff are active in shaping policy, funding and strategy within the wider scientific community as exemplified by the following examples:

##### Prizes and Fellowships

*Chemistry* staff have been awarded a number of prestigious fellowships and prizes since REF 2014 including: **Bos** was awarded an *International Academic Fellowship* from the Leverhulme Trust (2020); **Dalgarno** won the *RSC Sir Edward Frankland Fellowship* (2015) for "work in supramolecular coordination chemistry" and was made a *Fellow of the Royal Society of Chemistry* (2015); **Duncan** won the *Royal Society of Edinburgh (RSE) Senior Public Engagement Medal* (2018) for 'passionate and enormously productive advocacy for public engagement in Scotland, the UK and internationally'; **Hill** was the winner of the *Multiparty Collaboration Award* at the *Interface Scottish Knowledge Exchange Awards 2019*; **Jenkins** was awarded a *Barry Axcell Fellowship* (2015-18); Leslie was elected as *Fellow of the Royal Society of Biology (FRSB)* (2016); **Macgregor** won the *RSC Ludwig Mond Award* (2019) for 'computational studies of bond functionalization and activation'; **Maskell** was made an *Honorary Liveryman* of the *Worshipful Company of Brewers* (2018) and *Liveryman* of the *Worshipful Company of Distillers* (2019); **McKendrick** won the *RSC Chemical Dynamics Prize* for 'outstanding innovative research on the dynamics of molecules, including spectroscopy, kinetics or molecular interactions in the gas, liquid or solid phase' (2015); **Melchels** won the *Mid-career Investigator Award* from the *International Society of Biofabrication* (2019) and the *Dr Patrick Neill Medal for ECRs in the Life Sciences* from the *Royal Society of Edinburgh* (2019); **Schweizer** was elected as *Fellow of the Royal Society of Biology (FRSB)* (2020); **Stone** was elected as a *Fellow of the Royal Society of Edinburgh* in 2015 and was awarded the *RSC Toxicology Award* for 'contributions of chemical science to occupational and environmental toxicology'.

##### Collaborations

Staff in *Chemistry* have extensive active collaborations with groups at different universities and research organizations and industry both in the UK (>44 groups) and globally (>166 groups in > 31 countries across Europe, Scandinavia, Africa, Asia, Australasia and North America.

Some notable examples of the *international academic* collaborations that highlight the global reach and standing of our staff include: **Arrighi** and **McCoustra** with Mkongo (Ngurdoto Defluoridation

## Unit-level environment template (REF5b)

Research Station, Tanzania) resulting in 1 paper in *Adsorption*; **Barker** with Rehmann (University of Utrecht) and Zhou (University of Texas) resulting in 1 paper in *J Medicinal Chemistry*, **Bos** with Pollet (University of Bordeaux), resulting in 6 papers incl. *ASC Appl. Mater. Inter.*; **Bucknall** with Marder (Georgia Institute of Technology) resulting in 3 papers incl. *J. Mater. Chem. A*; **Costen** with Chandler (Sandia National Labs) and Aoiz (Complutense University of Madrid) producing a *Nature Chem.* paper; **Dalgarno** with Atwood (University of Missouri) resulting in 5 papers incl. *Nature Commun.*; **Euston** with Pappa (Democritus University of Thrace) in a H2020 grant resulting in 2 papers incl. *Biomolecules*; **Johnston** with Tantrakarnapa (Mahidol University, Thailand) resulting in 2 papers incl. *Environmental Health*; **Lee** with Bebbington (Montclair State University) in a joint grant resulting in a paper in *ACS Catal.*; **Macgregor** with Bertand (University of San Diego) producing a paper in *J. Am. Chem. Soc.*; **Maskell** with Speers (Canadian Institute of Fermentation Technology, Dalhousie University, Canada) resulting in 3 publications and a joint grant; **McKendrick** with Minton (Montana State University) with a joint grant resulting in 10 joint papers incl *J Am. Chem. Soc.*; **Melchels** has extensive collaborations with Malda, Dhert, Ablas, Gadella et al (University of Utrecht) including a joint grant resulting in 20 publications incl *Nature Commun.*, with Hutmacher, Klein et al. (Queensland University of Technology) leading to 2 joint grants and 9 publications incl. *Acta Biomaterialia*, with Lim and Woodfield (University of Otago) producing 3 publications and with Khademhosseini and Randolph (Harvard University) leading to 2 publications incl *Nature Protocols*; **L Paterson** with Nyk (Wroclaw University of Science and Technology) and Varma (Indian Institute of Science Bangalore) resulting in several papers incl. *Nanoscale*; **M Paterson** and **Townsend** with Sølling (University of Copenhagen) resulting in 4 publications incl. *Chem.Sci.* and with Stolow (University of Ottawa) producing 2 papers incl. *J. Chem. Phys.*; **Rickman** with Sugata (Toronto Western Research Institute) and Papadouplos (Queensland Brain Institute); **Schweizer** with Ugboogu (Abia State University, Nigeria) resulting in 2 papers incl. *FEMS Yeast Research*; **Stone** with Cassee (RIVM, Netherlands) resulting in 11 publications incl. *Scientific Reports* and *Nanotoxicology*) and Hristozov (University Of Venice) resulting in 7 papers incl. in *Nanotoxicology* and *NanoImpact*; **Vilela** with Xu (University of Hong Kong) resulting in 9 publications incl. *Appl. Catal. B Environ.*; **Welch** with Sivaev and Bregadze (Russian Academy of Sciences) resulting in 5 papers incl. 2 in *Dalton Trans.*

### Collaborating for Impact

Notable examples of *industrial* collaborations that include direct funding of research and through consortia include: **Bos** with Don (Semimetrics, UK) resulting in 3 papers incl. in *J. Mater. Chem. A.*; **Bucknall** with Fiscus *et al.* (ExxonMobil, USA) resulting in 2 directly funded projects and 3 publications incl. *Polymer*, as well as Kriegel (Coca Cola Inc, USA) resulting in 1 directly funded project and 3 publications incl. *Polymer*; **Coxon** with Kendall (Innoviphar Ltd, UK) resulting in a paper in *J. Pharmacy and Pharmacology*; **Euston** with Akintoye *et al.* (Marlow (Quorn) Foods, UK), Paul (Devro UK), van Damme (Mars plc, UK), MacKnight (Macphie of Glenbervie, UK) and Maganini (EcoTech Systems, Italy) in 3 UK and 1 H2020 projects; **Holmes** with Casey (Diageo Global Beer, Eire) resulting in 2 papers in *Food Science* and *Brewing Science*; **Hill** with Edinburgh Gin and Port of Leith Distillery through KTP projects; **Johnston** with BASF SE (Germany), Misvik (Finland), QSAR (Poland) in a H2020 project and Alissi Bronte SL (Spain), Vitiva dd (Slovenia), Martin Snijder Holding BV (Netherlands) in a EU FP7 project; **Lee** with Burns (Syngenta, UK) resulting in a paper in *Chem. Commun.*; **Leslie** with Ardron (Renishaw, UK) resulting in a paper in *Adv. Bio. Regulations*; **Mansell** with Hanton (Sasol Technology, UK) resulting in a paper in *Organometallics*; **L Paterson** with Pal (Tata Consultancy, India) resulting in a paper in *Scientific Reports*; **Stone** with Wohlleben (BASF SE, Germany) resulting in 5 papers incl. in *Nanotoxicology*;

**Willoughby** with Marlow Foods (Quorn), Diageo, Mars, Pennotec, Glenmorangie, and Scottish Leather Group.

## Journal / Book Editorships

Staff in *Chemistry* hold a number of **senior editorial positions** with a range of international journals including: **Barker** is a guest editor for *Molecules*; **Bos** is on the editorial boards of *J Phys. Energy*, *Sustainability*, and *Sustainability Chemistry*; **Bucknall** is on the editorial board of *Emergent Materials* and is a guest editor for *Plos One*; **Dalgarno** is on the editorial board of *Crystals*, was a guest editor for a special edition of *CrystEngComm* (2016), and was a volume editor for *Comprehensive Supramolecular Chemistry 2<sup>nd</sup> Ed.* (2015-17); **Duncan** is on the international editorial board of *J. Biol. Chem.*; **Euston** is guest editor for *Frontiers Sustainable Food Production* (since 2019); **Hill** is a member of the editorial boards for the *Journal of the American Society of Brewing Chemists*, *Journal of the Institute of Brewing, Fermentation, Food Control and Beverages*, she has also edited two books (*Brewing Microbiology and Spirit Production and Quality*); **Johnston** is an editor for *Nanotoxicology*; **Lee** is a member of the Advisory Board of the RSC's flagship journal, *Chemical Science*; **Mansell** was guest editor for special issue of *Inorganics* (2016); **McCoustra** serves on the editorial board for *Scientific Reports* and is guest editor of *Phys. Chem. Chem. Phys.*, **McKendrick** is a guest editor for *Annual Review of Physical Chemistry*; **Macgregor** is on the editorial board of *Structure and Bonding* and is on the advisory board of *Dalton Trans.*; **Melchels** has been guest editor for special issues in *Frontiers in Bioengineering and Biotechnology* and also *Bioengineering*; **Stone** is on the editorial board of both *Journal of Food Chemistry and Nutrition* and *Nanotoxicology*; **Schweizer** is an editor of *International Journal of Molecular Sciences*; **Willoughby** is on the editorial board of *Food and Bioproducts Processing*; **Yarwood** is the section editor-in-chief of *Cells*, on the editorial board of *Cellular Signalling* and on the advisory board of *Biochemical Journal*. He has also been guest editor for special editions of *Biochemical Society Transactions*; **Yiu** is on the editorial board of *Journal of Chemical Technology and Biotechnology* and has been guest editor a special issue of *Journal of Chemical Technology and Biotechnology*.

## International Conferences

Staff in *Chemistry* endeavour to raise visibility by being actively involved in the *organisation* of major international scientific meetings, representative examples of leadership in higher profile meetings include: **Costen**, **Greaves**, **McKendrick**, **Nahler**, **M Paterson** and **Townsend** organised the 28<sup>th</sup> *International Symposium on Molecular Beams* in Edinburgh in June 2019; **Macgregor** is on the 44<sup>th</sup> *International Conference on Coordination Chemistry (ICCC2020)* International Steering Committee and the International Chair of *SessionT20 – Computational and Theoretical Coordination Chemistry*; **L Paterson** has been a member of the *Photonex Scotland Conference* organising committee since 2015; **Stone** organized *Inhaled Particles XII* (Glasgow 2017); **Welch** is a member of the international organising committees for *International Meeting on Boron Chemistry (IMEBORON)* and *European Conference on Boron Chemistry (EuroBoron)*.

*Chemistry* staff have *chaired* >46 sessions at different international conferences and symposia including: **Bos** has chaired sessions at the *British Crystallographic Association Conference* (Lancaster, 2017) and (Warwick, 2018); **Bucknall** chaired the *ACI European PVC Industry Summit* (London, 2019); **McIntosh** chaired the 2019 *Scottish Dalton* regional meeting; **Stone** has chaired sessions at numerous international conferences and symposia including 2<sup>nd</sup> *International*



## Unit-level environment template (REF5b)

*Congress on Safety of Engineered Nanoparticles and Nanotechnologies* (Helsinki, 2015), and *Society of Risk Assessment* (Venice, 2017).

Chemistry staff are also recognised through numerous *invited*, *keynote* and *plenary lectures* at international meetings (>164 have been identified), with a few examples including **Arrighi** 6<sup>th</sup> *European Conference on Neutron Scattering* (Zaragoza, Spain 2015); *International workshop celebrating “50 Years of Neutron Backscattering”* (Munich, Germany 2016); **Barker** *RSC Symposium on Heterocyclic Chemistry* (Grasmere, UK 2019); **Bos** *MRS-J: Materials Research Meeting, Thermoelectric Symposium* (Yokohama, Japan 2019); *Royal Society UK – Korea research conference* (Chicheley, UK 2019); **Bucknall** *RSC Science to Enable the Circular Economy* (London, UK 2019), *European Masterbatch Summit* (Dusseldorf, Germany 2019), *American Physical Society National Meeting* (Boston, USA 2019), *American Chemical Society National Meetings* (Dallas 2014, Denver 2015 and San Diego 2016); **Costen** *33rd International Symposium on Free Radicals* (Tahoe, USA 2015); *Advanced Particle Imaging Techniques* (Telluride, USA 2016), *26th Conference on the Dynamics of Molecular Collisions* (Tahoe, USA 2017), *25th International Symposium on Gas Kinetics and Related Phenomena* (Lille, France 2018); **Coxon** *Novabiochem Chemistry and Biology of Peptides Symposium* (Durham UK 2017); *RSC Perkin Meeting* (St Andres, UK 2020); *EFMC Short Course on Kinetic Perspectives on Drug-Target Interactions* (Oegstgeest, Netherlands 2018); **Dalgarno** *International Seminar on Inclusion Compounds* (Walsaw, Poland 2015 and Kazan, Russia 2017), *RSC Macrocyclic and Supramolecular Chemistry Meeting* (Edinburgh, UK 2016), *9th Catalysis and Sensing for Our Environment Symposium* (Yangling, China 2019), *American Chemical Society Midwest Regional meeting* (2014); **Euston** *European Summit of Industrial Biotechnology* (Graz, Austria 2019); *Johnston 1st Interprofessional Education Nano Training School* (Venice, Italy 2019); **Lee** *RSC, ACS and GDCh “Transatlantic Frontiers of Chemistry” (TFOC)* (Kloster Seeon, Germany 2013), *9th RSC-CSJ Joint Symposium: Designing Molecular Function at the Nano-Scale* (London, UK 2018); **Leslie** *Advances in Biological Regulation* (Bologna, Italy 2014 & 2019), *European Symposium on Hormones and Cell Regulation* (Alsace, Germany 2014), *Tissue Engineering and Regenerative Medicine International Society Conference* (Kyoto, Japan 2018); **Macgregor** at *EuCOMC XXI* (Bratislava, Slovakia 2015) and *ICOMC* (Florence, Italy 2018), *VIII International School on Organometallic Chemistry* (Seville, Spain 2015), *Trans-Pyrenean Conference on Catalysis* (Toulouse, France 2016) and *USIC* (Glasgow, UK 2016); **Maskell** *Master Brewers of the Americas Association* (Jackonsville, USA 2015); **McCoustra** *Physique et Chimie des Milieux Interstellaire et Circumstellaire* (Marseille, France 2018), *American Chemical Society National Meeting* (Dallas, USA 2014); **McKendrick** *Stereodynamics* (St Petersburg, Russia 2014), *International Conference on Molecular Energy Transfer in Complex Systems* (Chengdu, China 2015), *RSC Spectroscopy and Dynamics Group Meeting* (Warwick, UK 2016), *RSC Awards mini-symposium on Surfaces and Interactions* (Oxford, UK 2016), *TSRC Workshop on Dynamics on Multiple Potential Energy Surfaces* (Telluride, USA 2014, 2016 and 2018), *Gordon Research Conferences* (Newport, USA 2017 and Easton, USA 2018), *International Symposium on Free Radicals* (Hayama, Japan 2017), *Faraday Discussion on Ionic Liquids* (Cambridge, UK 2017), *American Chemical Society National Meeting* (San Diego, USA 2019); **Melchels** *International Conference on Biofabrication* (Pohang, South Korea 2014, Utrecht, Netherlands 2015 and Würzburg, Germany 2018), *SELECTBIO Bioprinting & 3D Printing in the Life Sciences* (Cambridge, UK 2016); **M Paterson** *Novel computational methods for quantitative electronic structure calculations* (Kobe, Japan 2015); *Theoretical Chemistry and Computational Modelling in Europe* (Leuven, Belgium 2017); **Schweizer** *International Conference on Yeast Genetics & Molecular Biology* (Frankfurt, Germany 2013, Levico Terme, Italy 2015, Prague, Czech Republic

## Unit-level environment template (REF5b)

2017, Gothenburg, Sweden 2019); **Stone** *NanoTox* (Turkey 2014 and Germany 2018), *2<sup>nd</sup> EU-Asia Dialogue on Nanosafety* (Vienna, Austria 2018), *BioEM 2017* (Hangzhou, China 2017), *Society of Risk Assessment Annual Conference* (Venice, Italy 2017), *NanoSafe 2016* (Grenoble, France 2016), *Society of Risk Assessment World Congress* (Singapore, 2015), *Annual Graphene Summit* (Berlin, Germany 2015), *UK-U.S. Bridging NanoEHS Research Efforts Joint Workshop* (Venice, Italy 2015), *SRA Nano Risk Workshop* (Washington, USA 2014); **Townsend** *IoP Molecular Physics Workshop* (Caen, France 2015), *XLIC WG3 Meeting on Control of Chemical Reactivity* (Belfast, UK 2016), *Ultrafast 2018* (Edinburgh, UK 2018), *New Horizons in Chemical Physics* (Oxford, UK 2019); **Welch** *IMEBORON XV and XVI* (Prague 2014, Hong Kong 2017), *EuroBoron 7 and 8* (Suzdal, Russia 2017, Montpellier, France 2019), *INEOS-RAS 60th Anniversary Conference* (Moscow, Russia, 2014), *Pacificchem* (Hawaii, USA 2015); **Yiu** *ENM meeting on Carbon Nanostructures* (Honolulu, USA 2016), *3rd Intl Congress on Biosensor* (Ankara, Turkey 2016), *2nd Intl Conference on Materials Science and Nanotechnology* (Auckland, New Zealand 2017)

### Other Leadership and Recognition

**Barker** is a member of the *RSC Scottish Steering Group*, and is also an *Early Careers Network Committee Member for Scotland*; **Bucknall** has served as an *Adjunct Professor at Georgia Tech USA* since 2015 and also serves on the *STFC Facilities Access Panel* since 2018, acted as an expert witness for *3M (USA, 2015-16)* and consultant for *Church and Dwight (USA, 2018)*. He also served as the external examiner of *Imperial College MSc degree program in Plastics Electronics* (2017-2019); **Dalgarno** was an elected member of *RSC Dalton Division Council* from 2015 – 2018 and is a consultant for the *Cambrex Corporation* on molecular structural analysis; **Duncan** served on *STFC Science Board* (2015-18), the principal scientific advisory committee providing strategic oversight on all £670M research activities for STFC. He also currently serves on many international advisory panels and other UKRI panels, including for *EPSRC, MRC and STFC*; he also previously served on the *Executive Board of the Scottish Universities Physics Alliance (SUPA)*; **Euston** served as a committee member for the *SCI Agri-Food group* from 2015-2018 and served as external examiner for the *University of Teesside, School of Engineering Food Science* degree programs (2014-2018); **Hill** was external examiner of the *Leeds International Study Centre International Year 1 programme*; **Johnston** is a member of the *National Centre for the Replacement, Refinement & Reduction of Animals in Research (NC3Rs)* studentship evaluation panel; **Macgregor** is a member of the *EPSRC e-Infrastructure Strategic Advisory Board*; **Mansell** is a member of the *RSC interest group organising committee* for Main Group Chemistry; **Maskell** was given the *Freedom of the City of London* in 2019 in recognition of her 'Leadership in Brewing and Distilling'; **McCoustra** served as the chair of the *British Vacuum Council* (2016-19), is Member (since 08/2020) of the *Interdisciplinary Programme Advisory Committee (iPAC)* for GANIL (France), and is the *IUVSTA representative* (since 04/2020) on the steering group for 2022; **M Paterson** sits on the *ScotChem* (Scottish research and training pool for Chemistry) management board having taken over from **McKendrick**; **Melchels** is a scientific advisor for *Tessenderlo Group* (Belgium) which focuses on agriculture, valorizing bio-residuals and providing industrial solutions; **Rickman** sits on the Executive Board of the *Scottish Universities Life Sciences Association (SULSA)*, having taken over from **Duncan**; **Schweizer** serves as an Adjunct Professor of Biochemistry at *Friedrich-Alexander University, Germany*; **Stone** sits on many Advisory Boards including for the *EU Nanomedicine Characterisation Laboratory* and has been recognized as being in the top 1% cited researchers in the *Clarivate Analytics Highly Cited Researcher List* in the field of Toxicology since 2015; **Vilela** was recently named as the *Emerging Investigator in Flow*

## Unit-level environment template (REF5b)

*Chemistry for 2020* by the Journal of Flow Chemistry; **Willoughby** serves in multiple leaderships roles including Chair of *Scottish Industrial Biotechnology Development Group*, member of the *Scottish Biorefining Strategy Group*, and is deputy-chair of the Scientific Advisory Board of *Industrial Biotechnology Innovation Centre (IBioIC)*.

**Government Panels / Activities**

**Duncan** was part of the Scottish Government mission to Beijing, Shanghai and Hong-Kong led by the First Minister (April 2017) and a similar mission to showcase UK Science to Delhi and Bangalore, led by the Scottish Deputy First Minister (November 2019). He has also served as a member of the *Scottish Parliamentary Cross-Party Group for Life Science*. He is currently on secondment with *UKRI* and serves as *Director of Talent and Skills*; **Hill** served as a member of the Scottish Parliament *Cross-Party Working Group for Scotch Whisky* (2018-19).