Institution: University of Aberdeen

Unit of Assessment: 8 (Chemistry)

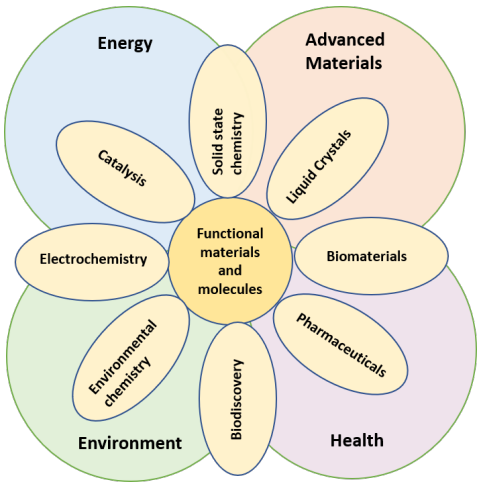
1. Unit context and structure, research and impact strategy

Introduction and Unit Structure

We are an outward looking, vibrant and diverse department with a strong international collaborative profile that has grown significantly since REF2014.

We engage and work with multiple partners (academic and industrial) to enhance the scope and impact of our research. We have been highly successful in obtaining funding from a diverse range of sources and have a high level of collaboration with other Schools within the University, particularly Engineering, Biological Sciences and Medicine, Medical Sciences and Nutrition.

Our main research strengths are shown below:



This submission comprises 20 research active staff, distributed over four overlapping research themes:

Health (**Storey, Jaspars, Deng, Ebel, Trembleau, Plater, Houssen**).

Environment (**Feldmann, Krupp, Raab, Cuesta**).

Energy (**Cuesta, Howe, Macphee, McCue, Mclaughlin, Skakle, Wildman**).

Advanced Materials **(Gibson, Howe, Imrie, Law, Mclaughlin, Skakle, Storey, Wildman)**.

The Department of Chemistry is part of the School of Natural and Computing Sciences. Departmental research activities are managed by a Research Committee chaired by the Director of Research (DoR) (*Mclaughlin*) with leaders from the four research themes (*Imrie, Jaspars, Feldmann, Cuesta* and the Head of Department (*Storey*)). This group formulates and implements research strategy and co-ordinates funding applications. Staffing strategy and budgets are overseen by the School. The Departmental Research Committee reports to the School Research Committee, which, in turn, reports to the institutional Research Committee. As DoR for the School, Cuesta is a member of the institutional committee.

Research Strategy

i) Significant Achievements Since REF2014

Our research income has grown from GBP11.2M in REF2014 to GBP26.7M, and our income-in-kind has almost doubled from GBP1.2M to 2.25M. We have increased our PGR numbers from 30 in July 2013 to 45 in July 2019, evidencing a strong upward trajectory of the Department's research vitality. We recruited two early career researchers at lecturer level and an EPSRC early career

fellow. New staff constitute 15% of the submission. There has also been significant procurement of new equipment (> GBP4M) across all themes. The award of two recent EPSRC New Horizons grants reflects the transformative, novel and adventurous character of our research and its potential to shape the future research landscape.

Since 2014 three spin-out companies (TauRx, Sirakoss and Enocell) have achieved further investment, growth and research impact, with continued collaborations with the Department. In 2020, Sirakoss was acquired by the Swedish firm OssDsign for more than $11M. A new spin-out company, GyreOx Pharma was launched in late 2019 with funding from Innovate UK and other investors. We have sustained and established new links with industry.

Achievements within the different research themes are:

***Health*:** The strategy has been to strengthen the link between discovery, synthesis and biosynthesis of molecules with biological and medical significance. New research in biosynthesis (*Deng, Ebel, Jaspars, Houssen, Trembleau*) has led to the key discovery of novel molecule families active against epilepsy and Alzheimer's disease (AD) in animals. Research with TauRx Therapeutics Ltd (led by *Storey*) has been highly successful in developing treatments and diagnostic agents for AD, resulting in six patents since 2014. It is the largest project in the University, running for almost two decades and currently employs 25 researchers (mostly PDRFs) in the Department. The project is interdisciplinary including researchers in Applied Mathematics, the School of Psychology and the Institute of Medical Sciences (University of Aberdeen), London School of Pharmacy, UCL and the University of Sussex. A new improved drug has now been developed, which has gained regulatory approval to treat patients in phase III Alzheimer's disease and behavioural variant frontotemporal dementia clinical trials, comprising approximately 2500 participants (*Impact Case Study 1*).

***Environment*:** Research involves the development of elemental speciation and elemental bioimaging methodologies for solving topical problems in environmental sciences and biosciences. Research is highly interdisciplinary as demonstrated by the award of the Royal Society of Chemistry (RSC) Interdisciplinary prize to *Feldmann* in 2016 for the development of analytical systems to identify biological metal metabolites. Exploitation of the expertise and world class analytical facilities led to the design of affordable methods for low/medium income countries to control inorganic arsenic in their rice products (*Impact Case Study 2*). *Feldmann, Krupp* and *Raab* have developed a field-kit for arsenic testing, which has facilitated a new market for Malawian rice.

***Energy*:** Research is focussed on the synthesis and investigation of sustainable materials for photo- and electrocatalysis, heterogeneous catalysis and energy conversion and storage. The research expertise in electrochemistry and photocatalysis has resulted in the development of a visible light activated photocatalyst with very high nitrate selectivity for the treatment of atmospheric NOx, which was tested on the streets of Copenhagen (*Macphee*). Key advances have also been made in understanding the chemical factors that control the activity and selectivity of the CO_2 reduction reaction (*Cuesta*). *Mclaughlin, Skakle* and *Wildman* have synthesised novel ionic conductors and have made the discovery of dual ion conductivity in a hexagonal perovskite, which has potential application in intermediate temperature ceramic fuel cells and is becoming an emerging new research area.

***Advanced Materials*:** This theme brings expertise in materials synthesis and characterization to tackle important challenges in liquid crystals, electrical and magnetic materials and biomaterials. There has been great success in liquid crystal research (*Imrie, Storey*) during the review period including ground-breaking research on the twist-bend nematic liquid crystal. This research has resulted in the award of the prestigious G.W. Gray Medal of the British Liquid Crystal Society to *Imrie* in 2019, which is awarded for outstanding research contributions of international quality in the field of liquid crystal science. Other key advances include pioneering a powerful new synchrotron radiation FTIR microspectroscopic technique (*Howe*) and the development, through the spin-out company Sirakoss Ltd, of Osteo3, a nanosynthetic bonegraft substitute designed to improve patient healing (*Gibson, Skakle*).

ii) Relationship to REF2014

Since REF2014, we have restructured the Department into four research themes based on our unique research strengths, vitality and critical mass (*Energy*, *Environment*, *Health* and *Advanced Materials*). Our strategy has been influenced by the Institution's strategic plan, Aberdeen 2040 (see REF5a). Our approach is to maximise our research potential by focusing on people, collaboration and enhancing our impact. Our overarching goal is to grow our world class activities in all four research themes. Our strategic aim is to increase research in *Energy*.

People: A strategic objective from REF2014 was to grow oil and gas and energy research. This strategy evolved to growth in energy futures. We made strategic appointments in the energy theme (*Wildman* (ionic conductors) and *McCue* (catalysis)). Another objective has been to increase the number and quality of postgraduate researchers (PGRs) to enhance our research. This has been facilitated by the allocation of University Elphinstone scholarships, which pay the fees of first-class PGRs and School of Natural and Computing Science studentships (a co-funding 50:50 model between the School and industry or other institution). We have broadened our international links and the diversity of PGR students with several PGRs being co-supervised with international partners. We also maintain a diverse staff base as described in section 2.

Collaboration: Interdisciplinary research (IDR) has been a major feature of the Department's research strategy since REF2014 and our ambition has been to expand IDR both within the University of Aberdeen and externally. The complementarity of the four core research themes provides an excellent basis for research collaborations with other disciplines, in particular, Engineering, Biological Sciences, Environmental Sciences, Physics and Medical Sciences. The IDR strategy has been facilitated by the University, driving interdisciplinary collaboration through the Grants Academy, offering sandpit events and workshops (see REF5a). To further promote inter- and intradisciplinary research we have actively participated in Scottish Funding Council (SFC) pooling initiatives such as ScotChem, Scottish Universities Life Sciences Alliance (SULSA), Energy Technology Partnership (ETP) and the Industrial Biotechnology Innovation Centre (IBIOC). This approach has been highly successful and 40% of our submitted outputs meet the REF definition of interdisciplinary research. We have also expanded our collaboration with industry with an average income from industry per FTE per year of GBP133k. Increased international collaborations have also been enabled by prioritising participation in European Commission, Newton, Commonwealth and GCRF research grant calls. As proposed in REF2014, we have facilitated staff contributions to national and international conferences and to visit potential collaborators by provision of annual departmental discretionary research funds to all staff.

Impact: A main element of our impact strategy over this REF cycle has been to support and grow the existing spin-out companies. This move is aligned with the regional economic development strategy to diversify the economy and reduce reliance on oil and gas and to encourage academic staff to form new spin-out companies. This has been supported by the University's Impact and Knowledge Exchange Team that assists in the setup of spin-out companies alongside the management and protection of intellectual property (see REF5a). Our impact has been further stimulated by the secondment of three staff (*Gibson, Storey, Macphee*) to their spin-out companies. We have benefited from the creation of a new position of 'Impact Champion' within the School. The post holder has organized workshops and events to promote and share best practice on impact generation. Staff have been encouraged to develop links with industry through knowledge transfer partnerships, Innovation Centres, personal contacts and through liaison with the University Industry Partnership Officer. By using our unique research expertise, we have endeavored to influence policy with government and non-governmental organisations (NGOs) as described, for example, in *Impact Case Study 2*. Further impact has been delivered by dissemination of our research to the media and public with support from the University's Communication Team and the Public Engagement with Research Unit (PERU).

iii) Future Research and Impact Strategy

- Our research strategy will remain closely aligned to that described in the University of Aberdeen's strategic plan, Aberdeen 2040. Chemistry will play a critical role in the Energy

Transition, Health, Nutrition and Wellbeing and Environment and Biodiversity interdisciplinary challenges. Staff will participate in University workshops, grant schemes and collaborative research opportunities that arise to further enhance our interdisciplinary research, sustain our PGR population and make new links with industry.

- We will build on our international research networks by instigating new collaborations via international collaborative funding such as UKRI International Collaboration, future EU schemes, Newton, Commonwealth and GCRF calls and by participating in University strategic partnerships with international institutions.
- We will sustain our existing partnerships and make new collaborative links with industry by participating in Knowledge Transfer Partnerships and other Innovate UK grants, pooling schemes such as ETP and Innovation Centres such as IBIOC and through liaison with the University Industry Partnership Officer.
- TauRx is co-located in the Department and aims to expand by 10% in the next five years with anticipated research funding of GBP12.3M. Research will concentrate on second generation molecules and new molecular discovery for treatment of Alzheimer's disease. A further strategic aim is for expansion of the two remaining spin-out companies Enocell and GyreOx.
- To grow our excellent research and impact, we will invest in further high specification instrumentation by securing funds through UKRI strategic equipment awards, collaboration with industry and University investment.
- Alongside the high-quality research described in the previous themes, we have identified three Aberdeen future Chemistry challenges, which will have transformative research impact. These challenges will shape our research portfolio in the themes of *Advanced Materials* and *Health* over the next 5 years and will enable new frontiers of chemical discovery.
  1) We aim to confirm and exploit the first observation of many body localisation (MBL) in the solid state. MBL systems can be used to protect quantum memory, allowing the tantalising possibility of performing topological quantum computation at finite temperatures. This project will be funded by the EPSRC New Horizons call (*Mclaughlin, Wildman*).
  2) A novel liquid crystal phase, the ferroelectric nematic phase (N_F) will be investigated. The N_F phase could lead to the next generation of extremely fast switching liquid crystal displays operating at lower power and has potential to transform the liquid crystal display industry. This project will be funded by the EPSRC New Horizons call (*Imrie, Storey*).
  3) We will advance the prediction of how gene clusters generate microbial natural products by connecting the mass spectrometry data of microorganisms directly to the gene clusters to simplify compound structure determination. This will enable us to manipulate these gene clusters more easily to generate novel bioactive compounds, with future application as pharmaceuticals. This project will be funded by EU Horizon 2020 involving chemists, micro and molecular biologists and industry (*Jaspars, Ebel, Deng, Houssen*).

Open Research

The University of Aberdeen is part of the UK Reproducibility Network and we implement an open and reproducible approach to research in which research papers and data are made available to the scientific community and the general public (see REF5a). In accordance with the University of Aberdeen's Open Access policy, researchers publish outputs using Green Open Access wherever possible. In 2020, 87% of all Chemistry's journal articles were compliant with the REF open access policy requirements compared with 24% in 2013. We also deposit research outputs in the public domain, prior to publication, on open access archives such as ChemRxiv and arXiv. All staff have an ORCID iD.

The University has a policy for Research Data Management and all PIs now include a data management plan in research proposals. We comply with the UKRI open data mandate as described in the Concordat for Open Data.

Research Integrity

As part of their commitment to research integrity, the University of Aberdeen has signed the San Francisco Declaration on Research Assessment (DORA) and provides mandatory Research Governance and Ethics training to all staff and PhD students involved in research. The University

of Aberdeen Research Governance Handbook provides a framework for research ethics and governance at the University. As a Chemistry unit we also follow the "Code of Practice" of the UK Research Integrity Office, which incorporates the key points of good practice at all stages of a research project. We have several internal procedures in place to ensure research integrity (ethical review of experiments, data management and UKRIO research checklist) in accordance with the UUK Concordat (2019) and report to the University's Research Policy Committee (RPC) on compliance with the Governance Handbook (see REF5a).

2. People

i) Staffing strategy and staff development

Demographic: We have sustained our staff numbers (20 staff), and retiring staff have been replaced. Staff appointed at professorial or reader level account for 65% of the total, and the mean and median ages are 51.5 and 52.5 years respectively. All category A staff are on substantive contracts. We envisage one full time retirement in the next five to six years and proleptic appointments will be made in accordance with our future research strategy.

Strategy: We recruit staff to enhance, complement and extend our existing expertise within the research themes and to create further interdisciplinary collaborative opportunities. Each appointment requires a business case to the School. Over the REF period our strategic goal has been to expand research in the Energy theme, and we have appointed two early career researchers at the lecturer level to balance the age profile and enhance the vitality of the Department.

Academic staff: *Wildman* was appointed in 2019, bringing a new research direction in local structure studies of solid electrolytes. The recruitment of *McCue* in 2019 allows continuing cutting-edge research in heterogeneous catalysis and further collaboration with Engineering following the retirement of Jim Anderson. *Houssen* was awarded an EPSRC early career fellowship in the health theme in 2019. He is working between the Department of Chemistry and the Institute of Medical Sciences, further promoting interdisciplinary research.

ECRs are 10% of our submission and are supported by being mentored on probation for three years, given reduced teaching loads, allocated a PGR student, start-up funds and travel support to attend conferences and meetings. These measures are in place to help ECRs to develop their research profile and nurture their career development to more senior positions.

We facilitate exchange between academia and industry by seconding staff. *Gibson, Macphee* and *Storey* are all partially seconded to spin-out companies demonstrating a significant investment in knowledge exchange (15% of the submission).

We hold whole Departmental research away days to refine research strategy and foster collaboration. Administration and teaching relief for all research active staff has been provided through the appointment of three staff on the teaching and scholarship career track.

Career Development

Training: The University's Researcher Development Unit (RDU) delivers courses designed for all career stages and includes PI development programmes, leadership and management training and mental health awareness. Researchers are allocated 10 days' professional development time per annum pro rata which enhances our research sustainability and vitality. This is formalised by the adoption of the Concordat to Support the Career Development of Researchers (2019) (see REF5a). All staff complete mandatory training in equality and diversity, research governance and ethics and information security. There is mandatory supervisor training for all new supervisors of PGRs and updates for experienced supervisors, which must be undertaken every five years. There is also data management and Open Data support through the library and IT services.

The Grants Academy (GA) supports researchers in all stages of the research grant cycle (see REF5a). The GA supports impact, interdisciplinary research and challenge led research under GCRF and Newton funding calls. Staff have benefited from impact pump priming funding to facilitate the impact described in *Impact Case Study 2* (*Feldmann, Krupp, Raab*) and to run a workshop (with researchers from the School of Law) to provide advice to the United Nations for

developing a new 'Ocean Treaty' to conserve and sustainably use marine biodiversity (*Jaspars*). The GA supports our spin-out companies and has protected intellectual property (*Gibson, Skakle*). Staff have undertaken impact training and attended impact workshops at both School and University level. Public engagement acts as a steppingstone towards impact and this has been supported by PERU (Section 4).

Academic staff: All academic staff undergo annual review. The individual's objectives, development and support requirements for the coming year are mapped onto the University of Aberdeen's Framework of Academic Expectations (FAE). Support and guidance are given on funding and multidisciplinary research opportunities alongside leadership and management training. Workloads are monitored at annual review and advice on promotion is given.

The FAE and promotions criteria include knowledge exchange (KE) and impact outcomes. Chemistry has significant engagement with KE and many of the staff's achievements beyond academia have been recognised. Staff who are successful at research and impact have a reduced administration load to increase their research time and are rewarded through promotion. The vitality and achievements of the research groups over the assessment period are reflected in promotions: (*Cuesta, McLaughlin* and *Skakle* to Professor; *Deng, Ebel* and *Krupp* to reader; *Trembleau* to senior lecturer; *Houssen* and *Raab* to senior research fellow). Since REF2014, 69% of eligible academic staff (FTE) have been promoted.

PDRFs: Our postdoctoral research fellows undertake annual interviews to progress their career development. The RDU offers training suitable for a wide variety of careers. Since 2014, fifteen PDRFs and/or PGRs have secured fellowships or academic positions at institutions around the world including Xiamen University, University of Missouri and the University of Bremen.

Research Leave: The University's research leave policy was updated in November 2019 and allows research leave for up to one year (see REF5a). Selection is based on the strength of the individual's research profile. Teaching can also be blocked into one semester to provide time to spend on research, research grant applications, outputs and impact. *Feldmann* and *Krupp* have had their teaching blocked into the first half session to enable research leave at the University of West Indies. *Feldmann* and *Macphee* have also held visiting professorships at Universidade Federal de Santa Catarina and Wuhan University of Technology, respectively.

ii) Research students

One of the unit's strategic goals is to increase the number, while enhancing the already high quality of our PGR students. The large increase in research funding since 2012/13, together with the introduction of University Elphinstone PGR scholarships, has resulted in a marked expansion of the PGR population. The number of PGRs has increased from 30 FTE in 2013 to 43 FTE from 2015/16 onwards (Table 1). The modest reduction in PGR numbers in 2019/20 is attributed to the impact of the Covid-19 pandemic and we anticipate an increase through deferred entry in 2021.

	12/13	13/14	14/15	15/16	16/17	17/18	18/19	19/20
PGRs registered (FTE)	32	31	35	43	43	44	43	35

Table 1 PGR numbers (FTE) registered in Chemistry over the whole year.

PGR Funding Mechanisms

All staff supervise research students. The recruitment of PGRs is achieved via the Postgraduate Research School, which is responsible for the progression and career development of all PGRs (see REF5a).

PGRs in Chemistry are supported by the Leverhulme CDT, the various Scottish Funding Council (SFC) research pooling initiatives (Section 1) and University Elphinstone studentships. More

traditional modes of studentship funding (Industrial CASE awards, DTG studentships) are also common, as well as examples of full industrial funding of studentships and European students supported through Marie Curie ITN, for example, MarPipe, (*Ebel, Jaspars*). There has been increasing funding from the British Council for Newton Studentships and Commonwealth scholarships (*Jaspars, Mclaughlin, Ebel, Deng*). In addition, a strategic partnership with Curtin University, Australia includes the funding of joint studentships (*Mclaughlin, Cuesta)*. We also have international studentships funded by the governments of Thailand, Saudi Arabia, Malaysia, Sweden and Brazil.

The School encourages industrial collaborations by offering matching funds for studentships when industrial funding is secured for the balance; examples include Innospec, DSM nutrition, SCG Cement co LTD and Chevron.

Doctoral Training

Progression of PGRs is monitored through a system of six-monthly reviews and a progress report and oral examination, after nine months and 21 months, conducted by two members of staff not associated with the research project.

Training for PGRs is provided by the Postgraduate Research School, combining courses from the University's generic skills programme (designed for PGRs at the University of Aberdeen) with discipline-specific courses. At the beginning of their PhD, all PGRs complete an initial skills audit to create their Training and Development Roadmap. All students are required to present their work at research group seminars. At the annual Departmental Postgraduate Symposium, a poster is presented by all level 1 and 2 students, while final year PGRs give a departmental seminar. In 2020 a one-day PGR seminar was successfully held on Microsoft Teams. There was a mixture of male and female multinational presenters and prize winners.

PGRs have benefitted from attending online courses delivered by academics at other chemistry departments in Scotland via the Scotchem pooling initiative. Students attend funded external training courses such as the ISIS neutron training course and the MS course in Swansea.

Conferences, Seminars and Events

We have a vibrant seminar programme and all PGRs and staff participate in weekly research colloquia delivered by a diverse range of external speakers including internationally renowned RSC medal winners Professors Polly Arnold, Jean Marie Tarascon, Melinda Duer, Frank Marken and Javier Pérez-Ramírez. We often host researchers from other departments, which provides an excellent opportunity for PGRs and staff to learn about and become engaged in multi-disciplinary topics. PGRs attend interdisciplinary seminars hosted by the School and Institution. We have a vibrant Chemistry society (led by PGRs) which organises a range of events including a weekly tea club, monthly mystery lecturers and an annual ceilidh. These activities are attended by staff and students. Individual groups organise their own research seminars. Most PGRs have presented posters and talks at national and international conferences. The high-quality research of the PGRs has been recognised by the award of poster and/or oral prizes at national and international conferences across all themes. Both the Department and School provide travel assistance for PGR participation in conferences. Several PGRs have taken part in public engagement and outreach events such as the Aberdeen Schools Hydrogen Challenge and "I'm a scientist, get me out of here".

iii) Equality and Diversity

All staff undertake Equality and Diversity training. There is a range of University groups such as the senior female network, LGBT staff network, parents and carers network, the staff race equality network and the disability network. We have an internationally diverse staff with 46% of academic staff, 60% of PGRs and 30% of PDRFs originating from outside the UK. Our PGRs and PDRFs are recruited from all over the world, which increases our global research profile.

Chemistry is a very active member of the School's Equality, Diversity and Inclusion (EDI) group (*Skakle* (chair), *Ebel*, *Mclaughlin*, *Raab, Wildman*), which gained Athena SWAN (AS) Bronze in 2016. Several new policies have resulted from the EDI group, which benefit all members of staff. These include carer support for conferences, return to work sabbaticals (for maternity or long-term

illness), ensuring gender representation on hiring committees, creation of a neutral language guide, which supports female and LGBT staff and active promotion support and encouragement.

To support and develop our ECRs and PDRFs, we are working towards creating more junior networks and ensuring that an increasing range of PGR bursaries and scholarships are available for women and other groups.

Our female staff have been awarded institutional leadership positions. *Skakle* was Head of School during the assessment period and *Mclaughlin* is research lead for Chemistry.

The Department acknowledges the importance of accommodating the needs of staff to achieve a suitable work-life balance. For example, departmental meetings take place in core hours and we allow staff, PDRFs and PGRs to work flexible hours. During the COVID-19 lockdown periods, meetings were arranged at times suitable for staff with caring responsibilities.

There is no barrier to promotion for part-time or fixed term staff. *Mclaughlin* is 0.8 FTE due to childcare commitments and has been promoted twice during the assessment period. More than ten fixed term staff working on commercial research have been promoted since 2014. All the female academic staff submitted to REF2014 have been promoted in the review period. In REF2014, 18% of our staff submission was female, in this submission 25% are female. In addition, 47% of PGRs and 46% of PDRFs are female.

Outputs were selected based on quality and in compliance with the institutional Code of Practice. The percentage of outputs attributed to female staff is broadly in line with the female staff percentage, reinforcing the effectiveness of our equality and diversity policies.

Health and Wellbeing

All new staff and PGRs receive an induction to the Department including a Health and Safety talk and, during 2020, a presentation on the Covid-19 arrangements that allowed research to continue. There is also a School Health, Safety and Wellbeing Committee with representation from Chemistry.

Supervisors are encouraged to foster supportive relationships, whereby they can offer both academic and pastoral support including directing students to central-level support if needed. We held mindfulness workshops for both staff and students at the Departmental Postgraduate Symposium. During the lockdowns we added a “Mental Health During Covid-19” poster to our website and all staff have held informal weekly online meetings to ensure the PGRs and PDRFs were coping with the situation. All staff and students have access to free off-peak membership at Aberdeen Sports Village.

3. Income, infrastructure and facilities

i) Income

Our research strategy for securing funding from a diverse range of sources has resulted in a step change in research income (from GBP11.2M in REF2014 to GBP26.7M). The research income has resulted in high quality research outputs including papers in *Nature Materials*, *Nature Chemical Biology*, *Nature Chemistry, Nature Communications*, *Advanced Materials*, *Angewandte Chemie* and *JACS*, and 18 patents for a range of applications including a new proton conducting membrane, novel catalysts and treatments and diagnostic agents for Alzheimer’s disease.

Internationalisation and collaboration are key strategic priorities, and we have prioritised expansion of our international collaborations. This has resulted in more than GBP2.5M of new international collaborative funding via EU, Newton, Commonwealth and GCRF.

UKRI income has grown from 11% in REF2014 to 15% of the new total, showing an increased focus on challenge-based research alongside continued high levels of engagement with industry. Staff participate in large interdisciplinary collaborations funded by UKRI such as the EPSRC funded UK wide Catalysis HUB. *Howe, Mclaughlin* and *Wildman* use UKRI large scale facilities such as ISIS and Diamond and collaborate with the researchers at these institutions. Our income-in-kind has almost doubled from GBP1.2M in REF2014 to GBP2.25M.

A selection of journal covers from Chemistry research at Aberdeen.

We have a strong collaborative network with industry, which makes up 67% of our research income. Our annual research income from industry has trebled since REF2014. An exemplar is the TauRX project led by *Storey* (GBP15.6M research income over the period 2014-2020). A new improved drug has now been developed, which has gained regulatory approval to treat patients in phase III Alzheimer disease clinical trials. The Gulf Organisation for Research and Development also funded a 4-year interdisciplinary project on "Green Concrete" (Glasser and *Macphee*, GBP2.8M with the School of Engineering (2012-16)) to develop processes, which reduce carbon dioxide emissions during cement production by sequestering carbon dioxide into building materials.

Income from charities has increased. An exemplar of the success of our interdisciplinary strategy is the award for a centre for doctoral training from the Leverhulme trust (2017) for training in sustainable chemicals and materials (GBP1.05M), providing funding for 15 PGRs. This interdisciplinary CDT includes researchers from Chemistry (*Cuesta, Deng, Mclaughlin, Trembleau*) alongside researchers from Engineering, Ecology, Economics and Politics.

Our current grant holdings total is above GBP12M and on average GBP3.9M of grants have been awarded every year since 2014. Such sustained success evidences the research vitality of the Department.

ii) Infrastructure and Facilities

Institutional Infrastructure:

We are supported by R&I in the creation and protection of intellectual property, project finance planning, grant submission and review and knowledge exchange. Chemistry has been successful in acquiring three Knowledge Exchange vouchers from R&I, which have been used for impact activities, for example, in running a workshop to provide advice to the United Nations to develop a new 'Ocean Treaty' to conserve and sustainably use marine biodiversity of areas beyond national jurisdiction. A case study describing the impact arising from this work will be submitted to UoA 18 (Law).

The curation of research outputs and data is supported by staff in the Library. Publications that arise from research undertaken in the Department are deposited in the institutional repository (AURA). Research datasets are stored within the repository function of Pure and made publicly available through the institutional research pages in addition to data published on other platforms, such as Dryad and Figshare.

Research data management is supported by IT Services. Our research groups also use shared drives where data can be accessed and validated between groups. The University allocate

research groups 2 Terabytes for this purpose (see REF5a).

Technical Staff

There are four full time technicians in Chemistry who take care of glassblowing, maintenance and upgrades of the equipment in the molecular analysis, elemental analysis, thermal analysis and X-ray diffraction facilities and are essential in training new users and supporting PGRs.

PGRs

The University has provided more than 20 PGR scholarships (Elphinstone, DTG and collaborative industry studentships) underpinning the increased number and quality of PGRs within the Department.

Departmental Infrastructure:

Significant investment has been made since 2013 with procurement of new equipment and refurbishment of the Marine Biodiscovery Centre, Japp and Thomas Clark laboratories, valued in excess of GBP4M.

Health

There has been significant investment from TauRX in equipment (GBP1.5M) including four Agilent HPLC instruments, three Waters Xevo LCMS instruments, two Agilent HS-GC-FID and one Agilent ICP-MS. This equipment is used to create data underpinning excellent outputs, patents and non-academic impact in successfully developing treatments and diagnostic agents for Alzheimer's disease as described in *Impact Case Study 1*. This equipment may also be used by research staff and students outside the TauRX project.

The Department provides a Molecular Analysis Facility, which is managed by *Jaspars*. This facility supports users from other institutions and schools, fostering collaboration. The Marine Biodiscovery Centre was refurbished during the review period and the spectroscopic equipment updated. The new equipment includes a Bruker 600 MHz NMR with liquid nitrogen cryoprobe, a Bruker 400 MHZ NMR, Orbitrap and MaxisII organic LC-MS and 2 triple quadrupole ICP-MS systems, totalling GBP1.6M.

Environment

The Elemental Analysis Facility managed by *Feldmann* and *Raab* has resulted in over 50 new collaborations worldwide from academia and industry using the high-specification instruments. The instrumentation includes several inductively coupled plasma mass spectrometers (ICP-MS and ICP-MS/MS) from Agilent for elemental analysis. The online simultaneous use of LC detectors was developed at Aberdeen and is still unique in the UK (*European Award for Plasma Spectrochemistry* (2015)). The equipment in the Elemental Analysis Facility was instrumental in developing the impact described in *Impact Case Study 2*. The laboratory is a partner laboratory of Agilent Technologies (USA) that supplies and renews an ICP-MS (approximate value GBP200k) as part of this agreement. The laboratory is supported by instrument manufacturer PS Analytics (UK) and Postnova (Germany) and a Postnova asymmetric flow field-flow fractionation instrument has been on loan from them since 2016 (GBP200k).

Energy* and *Advanced Materials

Materials Chemistry research is underpinned by a leading-edge thermal analysis laboratory overseen by *Imrie*. The laboratory's instruments were replaced recently with Mettler Toledo DSC2 and DSC3 differential scanning calorimeters, a Mettler Toledo TGA1 thermal gravimetric analyser coupled to a Hiden Mass Spectrometer for evolved gas analysis and a Mettler Toledo DMA1 dynamic mechanical analyser (GBP200k in total). These new acquisitions complement the existing facilities of polarised light microscopes equipped with heating and cooling stages. A commercial service is provided and used extensively by the oil and gas sector providing a key role in supporting the local economy.

Joint funding from the University and a private endowment resulted in the purchase of two new powder X-ray diffractometers (Panalytical Empyrean with Johansson monochromator and X'Pert powder (GBP250,000)), which were installed in 2014, creating a new powder X-ray diffraction

facility managed by *Mclaughlin.* There has been non-academic impact via research with external companies. For example, research has been performed with Rowan technologies to elucidate the origin of the red staining of Winchester Cathedral's roof.

Both research facilities are used by researchers in Engineering, Geosciences and Medical Sciences and researchers from the spin-out companies Sirakoss, Enocell and TauRX.

A new electron microscope facility opened in 2017 (GBP550 k) funded by the University. A Carl Zeiss Gemini 300 VP Field Emission Scanning Electron Microscope was installed. This forms the centrepiece of a new University-wide core facility named Aberdeen Centre for Electron Microscopy, Analysis and Characterisation and has been used extensively by staff in the themes of *Energy* and *Advanced Materials*.

There has been further investment by the University in the tier-3 High-Performance Computing facility "Maxwell": including GBP100k on hardware upgrades, GBP15-20k per annum on maintenance and support and GBP180k per annum on three support staff. This facility is essential for the research of *Law* for pioneering new research to gain further understanding of matter-antimatter collisions.

iii) Future Investment

A new GBP35M science teaching building is currently under construction. The ground floor of this building is dedicated to public engagement and outreach and will lead to better dissemination of cutting-edge research in the Department to the public and industry users.

The rolling programme of refurbishment of the Chemistry research laboratories will continue with particular focus on the Energy theme in line with the University's Strategic Plan Aberdeen 2040.

We anticipate further investment of GBP12.3M from TauRx in 2021 for further research in the Department developing new improved drugs for Alzheimer's disease (five years of 25 PDRFs, chemicals, consumables and new equipment).

An impression of the new Science hub adjacent to the world class Duncan-Rice library.

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

i) Collaboration

Internationalisation and collaboration are two of our key strategic priorities. We facilitate staff contributions to national and international conferences and opportunities to visit potential collaborators by provision of annual discretionary research funds to all staff and visiting fellow positions. We have attracted overseas visitors from China, Brazil, Canada, Chile, Ghana, South Africa, France and the Netherlands through a range of schemes including Erasmus, national research councils and foundations and CAPES. Further European links are established through the placing of final year undergraduate MChem students with European partners for research projects, with the reciprocal acceptance of Erasmus students for research placements with us.

International Collaboration: All staff have strong international connections. Since 2014, we have collaborated with colleagues in 50 countries resulting in over 300 joint publications. In 2019, 75.7% of Chemistry publications had at least one international co-author (WoS). We have led and been included in several international interdisciplinary EU grants (GBP1.7M), with industrial partners. For example, PharmaSea (*Jaspars, Ebel, Deng* with 24 partners), MarPipe (*Jaspars, Ebel* with 11 partners), Light2CAT (*Macphee* with five partners), SETNanoMetro (*Gibson* with 15 partners) ReMIND and Metrology for metalloproteins (Metallomics) (*Feldmann* and *Raab* with eight partners on both).

Key examples of collaboration are:

- The global reach of the liquid crystals group (*Imrie, Storey*) is evidenced by 33 papers published with international co-authors from 11 different countries. The significant collaboration with Lavrentovich and colleagues at Kent State University has resulted in eight papers and two patents. These describe electro-optic devices with potential applications in reflection displays, colour filters and tuneable liquid crystal lasers.
- The Environmental Chemistry group (*Feldmann, Raab* and *Krupp*) has published more than 100 papers since 2014 of which more than 70% are with international co-authors from 27 countries. The research is multidisciplinary with collaborators from the disciplines of Ecology, Archaeology, Medicine, Geology and Environmental Science.
- *Deng's* research (with *Jaspars, Ebel* and *Trembleau*) with Dr Kwaku Kyeremeh, University of Ghana, on the biosynthesis and chemical structures from Ghanaian soil and sediment bacteria has led to the discovery of antimicrobial agents leading to 24 publications and BBSRC funding. *Jaspars* subsequently acted as the UK PI for a MRC African Research Leaders Fellowship to Kyeremeh (GBP732,376 in 2018).

UK Collaboration We also have strong research collaborations with the Schools of Engineering, Biological Sciences, Geosciences and Medicine, Medical Sciences and Nutrition at the University of Aberdeen and between other UK Institutions. Collaborations have resulted in excess of GBP2.5M funding from UKRI, ERC and Scottish Enterprise. Specific examples include:

- Collaboration of *Jaspars* and *Houssen* with the structural biologist Naismith (Oxford) has led to the publication of 11 papers and an Innovate UK/BBSRC IB Catalyst award. Their research includes a complete understanding of all enzymes involved in the cyanobactin pathway at a structural level. This led to the engineering of two of the enzymes, which improved their potential for biotechnological applications and the formation of the spin-out company GyreOx.
- *Feldmann* has collaborated with the Aberdeen geologist Parnell and researchers from five other institutions to secure a NERC grant to investigate new approaches for production of selenium and tellurium for application in solar cells and to estimate future supply, leading to the publication of 16 joint papers.
- Research funding from the EPSRC UK Catalysis Hub for *Howe* has facilitated research collaboration with Lennon (Glasgow) using neutron spectroscopy to investigate zeolite catalysts (ten publications).

ii) Contribution to the economy and society

Our facilities and expertise are open and available to industry, via formal arrangements with individual companies, engagement in dissemination events and through research led PGT and CPD programmes.

Impact: We have strong links with industries that have funded or co-funded more than ten PGRs. The School co-fund these industrial PGR studentships to encourage collaboration with organisations beyond higher education. We have held research grants with 24 companies. Examples include Ingenza, AstraZeneca, Equinor, Johnson Matthey, Exxon Mobil, TauRx and Chevron. This has allowed our PGR population to grow and has provided opportunities for transforming fundamental research into impact through patents (18 patents have been granted since 2014).

The Department hosts four spin-out companies contributing to research impact:

Research with TauRx therapeutics (led by *Storey*) has continued to expand with GBP15.6M research income from 2014-2020. Research in the Department has resulted in a portfolio of chemistry-based patents and the manufacture of a drug for Alzheimer's disease that has been studied in two phase three clinical trials (and one that is ongoing) in 2,500 patients. In addition to chemistry design and development, the project has funded and operates a Good Laboratory Practice/Good Clinical Practice testing facility, the only one of its kind in a university department of chemistry in the world. This facility develops analytical methods for the detection of drug and metabolites in biological matrixes and is regularly inspected by the Medicines and Healthcare products Regulatory Agency.

The spin-out company Enocell Ltd was founded by *MacPhee* after research previously undertaken in the Department discovered a WO_3-based co-catalyst, which supports the low-potential oxidation of adsorbed CO. Their patented CO-tolerant anode technology is applied in low temperature fuel cells for portable electronics devices and to power generators for rural homes with limited or no access to grid power. Enocell has raised GBP2.3M in equity finance (2015-2019) and over GBP500k in UK/European grants (Scottish Enterprise SMART (2014) and Innovation Grants (2017) and Eurostars (2017)). The company has expanded to ten employees/contractors. Macphee is seconded 60% to Enocell.

Sirakoss Ltd founded by *Gibson* and *Skakle*, commercialises research on bone implant materials. Economic impact has been delivered through a ~GBP4M venture capital investment (November 2014-2018) and ~GBP2M of Innovate UK grants (2015 and 2018) to Sirakoss, and the company headcount has increased from two to seven people. Sirakoss Ltd was awarded the Venture Prize 2014 from the Armourers and Brasiers and received the CE Mark (2019) and US FDA 510(k) clearance (2020) for Osteo3, their nanosynthetic, bonegraft substitute designed to improve patient healing and be completely reabsorbed into bone. Sirakoss was sold to OssDsign for more than $11M in 2020. *Gibson* is seconded 40% to Sirakoss.

Biosynthesis research has led to the formation of a new spin out company GyreOx Pharma by *Jaspars* together with Naismith (University of Oxford) and Primrose (Entrepreneur) in 2019. GyreOx will use an automated chemoenzymatic process to treat complex diseases by producing designed compound libraries to hit 'undruggable' targets.

Influence on Policy: Further impact has been achieved via work with government and NGOs. Research in Environmental Chemistry (*Feldmann, Krupp* and *Raab*) established that rice contained high levels of inorganic arsenic and formed the basis of a recommendation to formally establish a maximum permissible level of the class I carcinogen inorganic arsenic in rice. Based on this recommendation, a maximum legal limit of 0.2 mg/kg has since been identified by the Food and Agricultural Organisation (FAO) of the United Nations and the World Health Organisation (WHO) and was implemented into EU law in 2016. Introduction of this limit into legal regulations of other nations has been initiated, most recently in Canada.

Jaspars has provided input into the UN treaty negotiations (the UN Convention on the Law of the Sea (UNCLOS) and the Convention on Biodiversity (CBD)) as advisor to the International Union for the Conservation of Nature, an intergovernmental organisation mandated by the UN.

The world-renowned analytical expertise of *Feldmann* and researchers resulted in a GCRF award for CAPABLE of GBP8M to seven organisations including the University of Aberdeen. This interdisciplinary project is assessing the exposure to air pollution and arsenic in food and water of around 100,000 people in Bangladesh and will link this exposure to mainly cardiovascular diseases and other non-communicable diseases.

Public Engagement:

Our staff have given several Café Scientifique talks, public lectures and participated in Aberdeen and the North East of Scotland's annual science festival, Techfest.

Particular highlights of public engagement are:

Skakle led the "Knit the elements project" where members of the public across the country knitted elements, which were then arranged into the periodic table, marking the International Year of the

Periodic Table as shown below. This project was supported by the RSC to create a "Stories of the Elements" Chatbot with which over 600 members of the public across the UK engaged.

Jaspars delivered the "Build a Medicine" activity at several locations including:

- The Natural History Museum (London).
- Explorathon 2014 (Association of Research Managers and Administrators award winning European Researchers' Night, Scotland) at which thousands of members of the public interacted with the project at Union Square Shopping Centre, Aberdeen.
- HMP Grampian in 2018 as part of Cell Block Science, the Wellcome funded Herald Higher Education Award winning project, which took science engagement into Scottish prisons. *Jaspars* delivered three engaging and innovative sessions for each category of prisoners.

Houssen led an initiative (funded by the RSC Outreach Fund) to inspire primary school children in both Chemistry and Biology. Experiments included the use of chromatin dyes to see chromosomes at different stages of mitotic division, and the isolation of DNA from fruits.

iii) Contribution to the research base

Research: Our researchers are highly cited with over 7000 citations since 2014 (WOS core collection) and have established new research areas. The demonstration of electrically induced tuning of the Bragg reflection in heliconical cholesteric mixtures by *Imrie/Storey* has triggered considerable research activity including the development of new devices (USA, China, Taiwan, South Korea). The discovery of significant ionic conductivity in hexagonal perovskite derivatives by *Mclaughlin, Skakle* and *Wildman* has led to new research in the area by groups in the UK, Japan and Italy with further new ionic conductors being reported.

Invited lectures: Our researchers' reputations have grown in the review period. Consequently, our researchers have received 20% more invitations to give keynote, plenary and invited lectures and seminars (in excess of 100 in the review period). *Feldmann* and *Imrie* have delivered plenary lectures at the 15th International Conference on Biogeochemistry of Trace Elements, China and the 17th International Ferroelectric Liquid Crystal Conference, USA respectively. *Imrie, Jaspars* and *Mclaughlin* have acted as discussion leader at or been invited to present their research at Gordon Research Conferences.

Leadership roles: Our staff have many leadership roles in the academic community. *Howe, Macphee, Skakle* and *Gibson* are all current members of the EPSRC peer review college. *Mclaughlin* and *Houssen* are associate members. *Deng* is a member of the BBSRC Pool of Experts. *Howe* and *Ebel* were members of the Norwegian Research Council peer review panel, Oslo in 2015 and 2016 respectively. *Imrie, Skakle* and *Jaspars* are members of the Carnegie Trust peer review panel.

Jaspars is currently vice-president international and a member of council for the Royal Society of Edinburgh (2019-2022). *Skakle* is chair of the RSC Solid State Chemistry interest group (2018-21). *Mclaughlin* was elected as secretary of the RSC Solid State Chemistry interest group (2014-17). She was also invited to serve on three international neutron diffraction facility access panels

during the REF period. *Cuesta* is Chair of Division 7 (Physical Electrochemistry) of the International Society of Electrochemistry.

Editorships: *Imrie* is editor of the journal Liquid Crystals (Taylor & Francis) and editorial board member of the journal Liquid Crystal Reviews (Taylor & Francis). *Feldmann* is an editorial board member for the Journal of Analytical Atomic Spectroscopy (RSC). *Cuesta* is a member of the Editorial Board of the Journal of Electroanalytical Chemistry (Elsevier). *Mclaughlin* was an editorial board member of the NPG journal Scientific Reports (2014-19).

Conference Organisation: Most staff have served on national or international conference organising committees. Key examples include the 27th and 28th International Liquid Crystal Conferences (Kyoto 2018 and Lisbon 2020), the World Biomaterials Congress (Glasgow 2020), the European Solid State Chemistry meeting (Glasgow, 2017) the European conference of Marine Natural Products (Glasgow, 2015) and the 14th International Trace Element Speciation Symposium (Aberdeen, 2014).

Fellowships: *Houssen* was awarded an EPSRC early career fellowship in 2019 (GBP1.3M) and *Mclaughlin* has been awarded a Leverhulme research fellowship commencing in 2021.

Awards and Prizes: *Feldmann* was awarded the RSC Interdisciplinary Prize in 2016 and the European Award for Plasma Spectrochemistry in 2015. *Imrie* and *Storey* became the first scientists to be awarded the prestigious Luckhurst-Samulski prize twice. This was awarded in 2017 and 2019 for liquid crystal research. This was followed up by the award of the 2019 G.W. Gray Medal of the British Liquid Crystal Society for *Imrie*. *Feldmann, Jaspars* and *Skakle* have been elected as Fellows of the Royal Society of Edinburgh.