Institution: EaStCHEM – University of Edinburgh (UoE)/University of St Andrews (UStA)

Unit of Assessment: UoA 8: Chemistry

1. Unit context and structure, research and impact strategy

1a. EaStCHEM overview and vision

For 15 years, EaStCHEM has united the Chemistry research schools of the Universities of **Edinburgh** (**UoE**) and **St Andrews** (**UStA**). Together, we form one of the largest Chemistry UoAs in the UK, comprising 89 academic staff at census date. Since 2014, we have published >3400 outputs with >45000 citations, awarded 526 PhD degrees, and secured >£113M in research income by spend, including >£9M from industry. EaStCHEM's vision is to provide a collegial, diverse, and stimulating environment in which to perform world-leading chemistry research that advances fundamental knowledge and solves global problems (Fig. 1). The excellence of our staff and the environment in which they work is indicated by 22 promotions (Section 2b) and external recognition from 40 national or international prizes/awards, the election of 9 staff as fellows to prestigious UK learned societies (Section 4f), and 13 ERC grants (Section 3a).

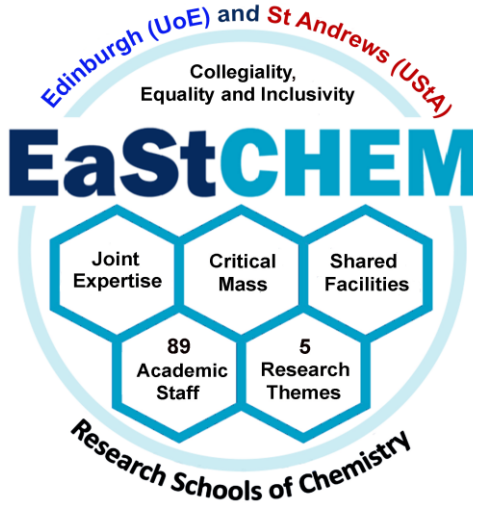

Fig. 1. *EaStCHEM at a glance.*

The following new initiatives, leveraged by our critical mass, have successfully reinforced our partnership.

- Creation of the **Christina Miller** and **Ettie Steele** Fellowships, which have provided the opportunity for five talented female postdoctoral researchers to establish themselves as independent group leaders, and improve our gender balance.
- Expansion of our world-leading research facilities, including the establishment of the *Electron Microscopy and Light Element Analysis Centre* (**Irvine**, EPSRC/**UStA**, £7.9M) and the *Scottish High Field NMR Centre* (**Uhrin**/**Ashbrook**, EPSRC, £1.4M).
- Delivery of major doctoral training programmes that combine high-quality research with skills development, including OPTIMA (Optical Medical Imaging, **Bradley**/**Colin Campbell**, EPSRC/MRC, £4.5M), CRITICAT (Critical Resource Catalysis, **Smith**/**Love**, EPSRC, £4.5M), and EaSICAT (East of Scotland Industrial Catalysis, **Smith**/**Thomas**, Industry/**UStA**/**UoE**, £2.5M).

EaStCHEM's longevity and sustainability attest to our shared values of collegiality, equality, and inclusivity that provide a firm foundation for our continuing partnership, and allow the exchange of best practice. Coordinated recruitment has built strength and complementarity, resulting in wide-ranging expertise across our joint research themes. Targeted investment has expanded the range of specialist pooled facilities accessible to all EaStCHEM researchers. Our synergy delivers collaborative research, training programmes, and joint funding opportunities. Integration across EaStCHEM has been reinforced through a *staff exchange seminar programme* (65 lectures since 2014, with staff from **UStA** visiting **UoE** and vice versa), *staff away days* (focusing upon research themes, interdisciplinarity, and funding), and the *EaStCHEM PhD Studentships Scheme* (£900k investment) involving PI co-supervision and research time at both **UStA** and **UoE**. Since 2016, the annual *EaStCHEM Conference for Early Career Researchers* has provided opportunities for collaboration and networking to post-doctoral research assistants (PDRAs) and early career researchers (ECRs).

1b. EaStCHEM research strategy

The development and implementation of research strategy is the responsibility of the EaStCHEM Board, composed of Heads of School (**Pulham**, **Morris**), Directors of Research (**Michel**, **Smith**), and Directors of Impact (**Uhrin**, **Zysman-Colman**), supported by **UStA**/**UoE** Research Theme Leaders. During this REF period, we targeted the implementation of three interdependent strategic

goals: (**1**) to *appoint and nurture* talented staff/ECRs, particularly those from under-represented groups; (**2**) to *stimulate and maximise* opportunities for collaboration with industry and other research end-users; and (**3**) to *focus and strengthen* our unifying research themes.

Goal (1) To *appoint and nurture* talented researchers across EaStCHEM

Recruitment of 29 academic staff (13 ECR Fellows, 9 Lecturers, 4 Readers and 3 Chairs) has strengthened the EaStCHEM research themes, established leadership in key areas, improved diversity, and increased staff numbers to 88.3 FTE (from 80.6 submitted to REF2014). Recruitment is aligned across EaStCHEM, ensuring that appointments have strategic value, with all panels having **UoE**/**UStA** representation. In response to an analysis of the diversity profile of recruitment during the REF2014 period, we created the **Christina Miller** (**CMF**) and **Ettie Steele** (**ESF**) Fellowships to support talented PDRAs from under-represented groups in the transition to independence. These schemes have resulted in five outstanding female appointments (**Garden**, **Jarvis**, **Hobday**, **Mey** and **Payne**), four of whom have subsequently obtained UKRI Future Leaders or Chancellor's Fellowships to establish themselves as independent group leaders (Section 2). Other ECR fellows (4 female and 4 male) contribute towards EaStCHEM's long-term sustainability (**Bell,** NERC Soil Security Fellow; **Erastova**, Chancellor's Fellow; **Gibbs**, UKRI Early Career Fellowship (ECF); **Ewen Campbell** and **Johnston**, Royal Society (RS) URF; **Yue**, UKRI Innovation Fellowship; **Kumar** and **Lancefield**, Leverhulme Trust ECF).

Goal (2) To *stimulate and maximise* opportunities for collaboration with research end-users

Our refreshed impact strategy (Section 1d) has raised the profile of impact-driven research, supported our staff to secure the time, funding, and skills to pursue impact goals, and provided increased opportunities for interaction with research users. This has generated a step-change in the level of end-user engagement by EaStCHEM researchers, and >£9M of industrial funding. Highlights include major partnerships with *BP*, *Infineum*, *Lubrizol*, *GSK, Sunamp* and *Eastman*; the creation of spin-outs *ZEMFuels*, *Invizius*, and *DESTINA*; and on-site hosting of companies including *Red-T/Invinity Energy Systems*, *The Falcon Project*, *LERC*, *MOFGen* and *Drochaid*. Staff interactions with industry have been strengthened by RS Industrial Fellowships with *Johnson Matthey* (**Wright**) and *Dr Reddy's* (**Clarke**), and the appointments of **Webb** (RS Industrial Fellow, former Chief Scientist at *Sasol*) and **Kirk** (industrial inorganic materials). UK and Scottish Government funding (>£30M) has secured the establishment of *GENESIS* (*GENE*ration *S*torage *I*nnovation and *S*ustainability Centre), a new business-facing facility for research and development focused upon batteries, hydrogen, fuel cells, and bioenergy.

Goal (3) To *focus and strengthen* EaStCHEM research themes

In 2015, after a consultation process with staff, we created five research themes (Fig. 2) that build on our excellence in fundamental chemistry, promote interdisciplinary research, and demonstrate our combined capability and strengths. These themes provide a coherent framework for collaborative research and impact, with each led by staff members from **UoE** and **UStA**. Three themes (**Catalysis and Synthesis**, **Chemistry-Biology Interface**, and **Functional Materials**) continue from REF2014, with a renewed focus to demonstrate their relevance to societal problems through impact. Of the new themes, **Structural Chemistry and Chemical Dynamics** encompasses recognized strengths in these areas, and **Energy, Environmental and Sustainable Chemistry** addresses the major global challenges of renewable energy, sustainable feedstocks, and environmental protection.

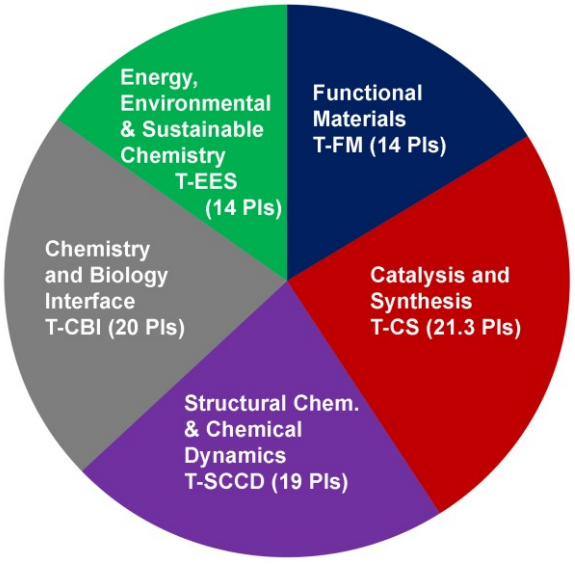

Fig. 2. *The EaStCHEM research themes.*

1c. Evidence of the success of EaStCHEM's research strategy across our themes

Theme – Catalysis and Synthesis (T-CS)

Leaders: **Cowley/Watson (21.3 PIs)**

Research strengths: main-group chemistry, biocatalysis, enantioselective catalysis, natural product synthesis, organometallics and metal-based/earth-abundant catalysis, reaction mechanism elucidation, fabrication of nanoparticles, and supramolecular chemistry.

Investment in people: **Ingleson** (Professor, main-group synthesis and catalysis); **Johnston** (URF, enantioselective catalysis); **Kay** (Lecturer from RSE Fellowship, nanomaterials); **Kumar** (Leverhulme Trust ECF, earth-abundant catalysis); **Stasch** (Reader, main-group synthesis); **Watson** (Reader, homogeneous catalysis); **Webb** (Reader, industrial catalysis).

Vitality and sustainability: ERC Advanced Grants (**Arnold**, **Lloyd-Jones**), Consolidator Grant (**Ingleson**), and Starting Grants (**Cockroft**, **Cowley**, **Lawrence**). Our strength in catalysis underpinned the CRITICAT CDT, which has trained over 80 PhD students (**Smith**/**Love**).

Highlights

- The Janus face all-*syn*-1,2,3,4,5,6-hexafluorocyclohexane was shown to be the most polar aliphatic compound (**O'Hagan**/**Philp**/**Slawin**, *Nature Chem.* **2015**).
- A detailed experimental, EPR, and computational study of the bicarbonate radical illustrates its extreme acidity and unique reactivity with lipids (**Buehl**/**Walton**, *JACS* **2015**).
- Detailed reinvestigations of protodeboronation reactions have overturned prior dogma, and led to mitigation of troublesome side reactions in key industrial processes (**Lloyd-Jones**, *JACS* **2016**/**2017**; *Nature Chem.* **2016**).
- A novel activation method provides a generic platform for the discovery of non-precious metal catalysis (**Thomas**, *Nature Chem.* **2017**).
- The demonstration that chalcogen bonding interactions are dominated by n-σ^* orbital delocalization (**Cockroft**, *JACS* **2017**) resulted in the enhanced reactivity of catalysts (**Smith**/**Slawin**/**Cockroft**, *ACIE* **2020**).
- A supramolecular Pd_2L_4 capsule performed as an efficient "*artificial Diels-Alderase*" (**Lusby**/**Lawrence**, *JACS*, **2018**).
- Sodium amide proved an excellent catalyst for allylic C(sp^3)-H bond activation of alkenes (**Schneider**, *JACS*, **2019**).
- The total synthesis of the alkaloid *brevianamide A*, an elusive target for over five decades due to its molecular complexity, was achieved in only seven steps using a bioinspired cascade reaction (**Lawrence**, *Nature Chem.* **2020**).

Collaborations and impact: major research partners include *AstraZeneca*, *GSK*, *Novartis*, *Syngenta*, *Lubrizol*, *Eastman* and *TgK Scientific*, who have provided >£2.5M in industrial support. Collaboration with *TgK Scientific* and *Bruker* commercialised the *InsightXpress* stopped-flow technologies for the analysis of fast reactions using *in-situ* IR and NMR spectroscopy (Fig. 3, **Lloyd-Jones**). Investment from *Eastman Chemicals* (£1.5M, **Clarke**/**Lloyd-Jones**/**Woollins**) led to catalyst development that solved an industrial problem now proven at pilot plant scale. The isothiourea HyperBTM catalyst is used on multi-kilogram scale by *Syngenta* (**Smith**).

Fig. 3. *InsightXpress reaction monitoring technology (***Lloyd-Jones***/Bruker/TgK Scientific).*

Theme – Functional Materials (T-FM)

Leaders: **Ashbrook/Morrison (14 PIs)**

Research strengths: magnetic and multiferroic materials, porous materials, energetic materials, optoelectronic materials, polymers, and synthesis using extreme conditions. By its nature, research in T-FM is applications-driven, with target materials employed for energy conversion and storage, gas separation, sensors, information storage, and cryogenic refrigeration.

Investment in people: **Cumby** (Lecturer, inorganic materials); **Gibbs** (UKRI Early Career Fellow, diffraction of materials); **Hobday** (Chancellor's Fellow from CMF, barocaloric materials); **McKeown** (Professor, organic porous materials); **Zysman-Colman** (Professor from EaStCHEM Fellowship, optoelectronic materials).

Evidence of vitality and sustainability: ERC Advanced Grants (**Attfield**, **Morris**) and Consolidator Grant (**Ashbrook**); EPSRC Senior Fellowship (**Morris**); EPSRC Platform Grant (**Attfield**, £1M); a grant to establish the Charles University Centre of Advanced Materials (**Morris**, €8M); and a US Defense Threat Reduction Agency grant (**McKeown**, $1.5M).

Highlights

- A new family of structurally complex zeolites, with embedded isoreticular properties, adsorb carbon dioxide selectively (**Wright**, *Nature*, **2015**), and 'unfeasible' synthetic zeolites were prepared using a new mechanism (**Morris**, *Nature Chem.* **2016**).
- Photoluminescent thin films of bismuth-based metal-organic hybrid materials are potential third-generation photovoltaics (**Payne**/**Irvine**, *Nature Commun.* **2017**).
- Membranes of polymers of intrinsic microporosity (PIMs) demonstrated exceptional performance as membranes for gas separations (**McKeown**, *Nature Mater.* **2017**) and redox-flow batteries (**McKeown**, *Nature Mater.* **2019**).
- The first pressure-induced transformation of a 2D precursor into a crystalline 3D zeolite, achieved at 1 GPa/200 °C, exemplified a powerful new technique for zeolite discovery (**Ashbrook**/**Attfield**/**Morris**, *J. Mat. Chem. A* **2018**).
- A general and practical method to obtain super-tetragonality and giant polarization using interphase strain in thin films was demonstrated (**Scott**, *Science,* **2018**).

Collaborations and impact: key partners range from SMEs (*5D*, *MOFGen*) to multinational companies (*Johnson Matthey*, *PQ Silicas*, *Teleflex*, *BP*, *Chevron*). Low-cost microfabrication enabled commercialisation of nanoelectrodes with ultra-high sensitivity and rapid response (**Mount** with *Nanoflex;* Fig. 4). Explosives that are safer to manufacture, transport and store have resulted from computational predictions of the intrinsic sensitivities of explosives to initiation by shock (**Morrison**/**Pulham** with *UK MoD*/*US DoD*). An impact case study (ICS) showcases how porous materials expertise (**Morris**/**Slawin**) led to commercialisation (*MOFGen*, *PanaceaNano*), and implementation of innovation policy in Sweden.

Fig. 4. *The Nanoflex electrode.*

Theme – Chemistry-Biology Interface (T-CBI)

Leaders: **Goss**/**Colin Campbell** **(20 PIs)**

Research strengths: medicinal chemistry, biological/medical imaging, natural product and analogue synthesis, the molecular understanding of protein structure and function, the investigation of enzymes and metabolic pathways, the chemistry of diseases including those that disproportionately afflict the world's poorest nations (microbial, parasitic, and genetic).

Investment in people: **Bode** (Lecturer from EaStCHEM Hirst Fellowship, biological EPR); **Clarke** (Chancellor's Fellow now Senior Lecturer, mass spectrometry); **Horrocks** (Lecturer, biophysical chemistry); **Jarvis** (UKRI Future Leaders Fellow from CMF, chemical biology); **Lilienkampf** (Lecturer, chemical biology); **Mey** (Chancellor's Fellow from CMF, modelling of protein structure).

Vitality and sustainability: ERC Advanced Grants (**Naismith**, **Bradley**), Consolidator Grant (**Goss**), and Starter Grant (**Michel**); EPSRC Centre for Doctoral Training OPTIMA (**Bradley**, £4.5M), EPSRC IRC Proteus (**Bradley**, £3.9M), and ARREST-TB (**Bradley**, EU, £4M) are developing revolutionary technologies for the optical detection of lung disease (Fig. 5); St Andrews Multidisciplinary Anti-infective Research and Therapeutics

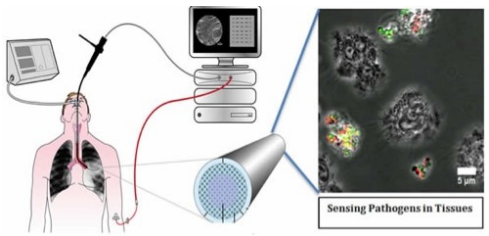

Fig. 5. *Imaging system to diagnose lung disease from Proteus.*

(SMART) Centre (**Goss**, RS/**UStA**, £750k); a GCRF award to provide antibiotic therapies in Africa (**Florence**, £900k).

Highlights

- A coiled-coil domain acts as a molecular ruler, with genetic manipulation allowing regulation of chain length in lipopolysaccharide production (**Liu**/**Naismith**, *Nature Struct. Mol. Biol.* **2015**).
- Ligand-based NMR was used to screen glycans for binding to blood protein factor H, suggesting sialic acid has a critical role in human renal complement homeostasis (**Uhrin**, *Nature Chem. Biol.* **2015**).
- The biosynthesis of high-value fatty-acid thioesters was achieved through site-directed mutagenesis of bacterial pimeloyl-CoA synthetase (**Naismith**/**Campopiano**, *Nature Chem. Biol.* **2017**).
- Super-resolution microscopy of single macromolecules is illuminating the role of protein aggregation in the development of Parkinson's disease. (**Horrocks**, *Nature Commun*. **2018**).
- Unnatural polymers have been prepared in cells via biocompatible free radical photopolymerisation, providing the ability to alter cellular motility, and to label cells by generating fluorescent polymers (**Bradley**/**Lilienkampf**, *Nature Chem.* **2019**).
- The first halogenase from a virus was discovered allowing characterization of a flavin-dependent halogenase with a preference for iodination (**Goss**, *Nature Chem.* **2019**).
- Stimulated Raman scattering microscopy is being utilised to study intracellular distribution of label-free ponatinib in live cells (**Hulme**, *J. Med. Chem.* **2020**).

Collaborations and impact: key partners include *AstraZeneca*, *Novartis*, *Invizius*, *Cresset*, *Ingenza*, and *Lucite*. *Edinburgh Molecular Imaging* is developing targeted fluorescent optical imaging agents as a diagnostic tool for colon cancer (**Bradley**). With Scottish Enterprise High Growth Spin Out Funding, **Goss** has established *XGenix*, a company focussed on providing bespoke halogenation solutions. *AstraZeneca* is using new MS methods for 3D imaging for screening of the distribution of drugs in cells (MS Facility Manager **Mackay**, Section 3b). *Cresset* has integrated new drug binding modelling methods into their pharmaceutical/biotech software for research customers (**Michel**/**Mey**). ICS highlights: (**1**) spin-out success providing direct detection of microRNA disease biomarkers (**Bradley**, *DESTINA*); (**2**) expert witness testimony leading to enhanced protection for biopharmaceutical patents (**Naismith**, *Amgen*); and (**3**) new companies generating therapies that control immune system response through factor H (**Barlow**/**Uhrin**, *Gemini* and *Invizius*).

Theme – Structural Chemistry & Chemical Dynamics (T-SCCD)

Leaders: **Baddeley**/**Alexander** **(19 PIs)**

Research strengths: diffraction techniques (particularly at elevated pressures), crystallisation, electron microscopy, surface and interface characterisation at single molecule resolution, theory and computation, ultrafast imaging and spectroscopy, and reaction dynamics.

Investment in people: **Ewen Campbell** (RS URF, astrochemistry); **Erastova** (Chancellor's Fellow, modelling of surfaces and materials); **Johansson** (Lecturer from RSE/BP Fellow, photo-induced molecular magnetism); **Payne** (ESF, structure of energy materials); **Seery** (Professor, chemical education); **Szabla** (Lecturer, computational organic chemistry).

Vitality and sustainability: EPSRC New Investigator Award (**Johansson**); BBSRC 17ALERT Award (**Clarke**); EPSRC Scottish High Field NMR Centre (**Uhrin**/**Ashbrook**, £1.4M); EPSRC Strategic Equipment Award (**Parsons,** £600k) to fund an X-ray diffractometer for extreme conditions; EPSRC Prosperity Partnership (**Camp**/**Pulham** with *BP*, £2.6M).

Highlights

- Remarkable enhancement of magnetic ordering temperatures for rhenium complexes was achieved by using pressure (**Brechin**/**Parsons**, *Nature Commun.* **2016**).
- High levels of cation disorder significantly improve quantum efficiency, stability and emission lifetimes for europium-doped nitridosilicate for use in white-light-emitting diodes (**Attfield**/**Zhou**, *JACS* **2017**).
- A novel organocatalytic methodology generated enantioenriched surfaces with functionalities

that are not accessible by other methods (**Haehner**/**Smith**, *ACIE* **2018**).

- Unprecedented insights into photochemical reactions were obtained from ultrafast X-ray scattering, using an X-ray free electron laser (**Kirrander**, *Nature Chem.* **2019**). This research on "*making the first molecular movies in quadrillionths-of-a-second frames to reveal the intricate structural dances of molecules as they undergo chemical reactions*" was selected by the US DOE as one of their research highlights from the last 50 years (Fig. 6).

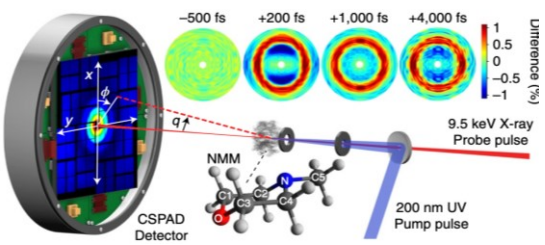

Fig. 6. *Determination of the structure of the excited state of N-methyl morpholine from ultrafast X-ray scattering.*

- A multi-state molecular switch based on the endohedral fullerene Li@C_{60} has been demonstrated (**Eleanor Campbell**/**Schaub**, *Nature Commun.* **2019**).
- Quantum chemical calculations elucidate the photochemical mechanism of the formation of prebiotic nucleosides necessary for the RNA/DNA-mediated origins of life (**Szabla**, *Nature* **2020**).

Collaborations and impact: characterisation of the role of additives at low concentrations during PVC manufacture resulted in a new formulation that has been produced globally on a tonne scale by *INEOS* (**Uhrin**/NMR Facility Manager **Bella**). **Schaub**'s work with *Integrated Graphene* provides a disruptive manufacturing process for high-quality 3D graphene foam electrodes. An ICS highlights how molecular simulation and high-pressure experimentation have transformed product development for major lubricant additive producers (**Camp**/**Pulham**).

Theme – Energy, Environment and Sustainability (T-EES)

Leaders: **Irvine**/**Kirk** **(14 PIs)**

Research strengths: new materials for photovoltaic technologies, energy storage (phase-change materials, lithium and sodium batteries, fuel cells, supercapacitors, membranes for redox flow batteries); processing of synthetic fuels (separation of gases and utilisation of CO_2, electrolysis, green ammonia, efficient hydrogen production); critical raw materials (valuable metal recovery via urban mining and sustainable polymers); and environmental analysis (air quality and peatlands).

Investment in people: **Bell** (NERC Soil Security Fellow, environmental chemistry); **Garden** (UKRI Future Leaders Fellow from CMF/Ramsay Memorial Fellowship, sustainable polymers); **Kirk** (Lecturer now Senior Lecturer, industrial inorganic materials); **Lancefield** (Leverhulme Trust ECF, renewable feedstocks); **Yue** (EPSRC UKRI Innovation Fellow, energy materials).

Vitality and sustainability: NEXGENNA Faraday Challenge Award (**Irvine**/**Armstrong**/**Morris**, £12M) to accelerate the development of high-performance sodium ion batteries; two EPSRC funded centres for Energy Materials "*Multiscale tuning of interfaces*" and "*Surfaces for energy applications*" (**Irvine**, £2.1M); EPSRC Critical Mass Funding for Emergent Nanomaterials (**Irvine**, £1.5M); EPSRC-JSPS Core-to-Core Programme (**Zysman-Colman**; £1M) based upon materials exhibiting highly efficient thermally activated delayed fluorescence; a GCRF grant "*Chemical recycling of electronic waste for sustainable material consumption in India*" (**Love**/**Morrison**, £400k).

Highlights

- Functionalised high-value phenols are obtained from an organo-solvated lignin through a two-step depolymerization (**Westwood**/**Lancefield**, *ACIE* **2015**), with aromatic monomers available in an acid-catalysed process (**Westwood**, *JACS* **2015**).
- Urban mining through selective extraction of gold from a mixture of metals was achieved by a simple ligand (**Morrison**/**Love**, *ACIE* **2016**).
- Electrolysis and fuel cells can be unified in a single, easily manufactured, device by preparing a solid oxide cell with an electrode coated with finely dispersed metal nanoparticles (**Irvine**, *Nature,* **2016**).
- Macrocycles containing three metal cations were shown to be efficient catalysts for ring-opening polymerisation to make sustainable polyesters (**Garden**, *Chem. Sci.* **2020**).

- A linear B,N-doped heptacene demonstrates multi-resonant thermally activated delayed fluorescence (**Buck**/**Slawin**/**Zysman-Colman**, *JACS* 2020).
- High proton and oxide-ion conductivities of hexagonal perovskites provide promising new materials for energy-related applications (**Savaniu**/**Irvine**, *Nature Mater.* 2020).

Collaborations and impact: **Irvine**'s work has attracted inward investment to establish the *Scottish Centre for Clean Energy Storage and Conversion and Enterprise Hub* (Fig. 7) with £30M of funding from the Tay Cities Deal. **Heal** provides expert advice to DEFRA's *Air Quality Expert Group* and the Department of Health's *Committee on the Medical Effects of Air Pollutants*. ICS highlights: (**1**) new phase-change materials that have enabled commercialisation of domestic heat storage (**Pulham**/*Sunamp*); (**2**) **Irvine**'s major role in the development of hydrogen as a fuel for public transport through policy and project implementation, culminating in the launch of the Scottish Government's *Hydrogen Accelerator*.

Fig. 7. *Site of the Scottish Centre for Clean Energy Storage and Conversion on the* ***UStA*** *Eden Campus.*

1d. Interdisciplinary research (see Section 4)

EaStCHEM's recognition of the importance of interdisciplinary research has: (**1**) guided strategic appointments; (**2**) led to new infrastructure initiatives; and (**3**) enhanced collaboration across our research themes, and with other disciplines, through PhD studentship funding. Our commitment mirrors that of both institutions regarding the importance of interdisciplinarity (see Institutional Environment Statements (IES), **UStA**/**UoE**, Section 2).

As examples of EaStCHEM's strategic appointments: (**1**) **McKeown** drives collaboration with **Chemical Engineering** on the development of highly permeable and selective polymer membranes for CO_2 capture; (**2**) **Zysman-Colman** and **Gibbs** broaden links with **Physics** on optoelectronic and inorganic materials; and (**3**) **Jarvis** brings additional expertise in biocatalysis at the Chemistry/Biology interface. Infrastructure initiatives such as the *Scottish High Field NMR Centre* (**Uhrin**/**Ashbrook**) provide Scottish researchers, across physical and biological sciences, access to cutting-edge liquid and solid-state NMR instrumentation. Support of interdisciplinary research extends to co-supervision of PhD students between disciplines (including Geoscience, Earth Science, Biology, Physics, and Engineering), with both **UStA** and **UoE** having dedicated university-led interdisciplinary PhD schemes. Institutional drive to promote interdisciplinarity has resulted in **Goss** leading an Engineering Institute at **UStA**, to focus on applied interdisciplinary research in the absence of an established School of Engineering.

1e. EaStCHEM impact strategy

EaStCHEM's refreshed impact strategy aligns with those of our institutions (**UStA**/**UoE** IES, Section 2) and has resulted in a clear step-change in staff involvement in, and achievement of, impact generation. We have built leadership and support through the establishment of an EaStCHEM Impact Team, with dedicated Directors of Impact (**Uhrin**/**Zysman-Colman**) and Impact Coordinator (**Fay Campbell**). The team promotes best practice and works closely with business development executives, public engagement and institutional impact support. In 2015, we established the *EaStCHEM Industry Advisory Board* (IAB), comprising senior executives from a range of sectors and including representation from large multinationals, SMEs and the public sector (*BP*, *Johnson Matthey*, *Bayer*, *Synthomer*, *West Brewery*, *Knowledge Transfer Network*, *ScotCHEM*). The IAB provides guidance on enhancing engagement with research users, feedback on proposed initiatives, and market intelligence about future trends and opportunities across a range of industries.

EaStCHEM impact strategy has focussed on the following three key objectives.

Objective (1) Raising the profile of impact

Increasing recognition of the fundamental importance of applying our research for wider benefit, and celebration of the research challenges that this can present, have resulted in a significant

culture change. This has been achieved through the following initiatives.

- Championing of impact by senior leaders from EaStCHEM at away days, symposia, and staff meetings.
- Incorporation of impact plans into annual performance reviews, resulting in workload adjustments to allow colleagues to dedicate time to impact.
- Inclusion of potential to generate impact as an important criterion for new appointments and career progression.
- Initiation (2018) of an industry speaker series to forge stronger links with industry. This has also directly resulted in successful collaborations (*AstraZeneca*, PhD studentship, **Zysman-Colman**/**Smith**; *Concept Life Sciences*, PhD studentship, **Goss**).

Objective (2) Supporting staff to develop impact

We have helped staff secure the time, funding, resources, and skills to pursue impact goals.

- EPSRC IAA funding of over £810k has supported 40 impact-based projects with links to 22 industrial collaborators, and involved 26 academic staff. Strategic use of these awards has led to ongoing collaborations and significant matched and follow-on industrial funding: £8.5k from *SST Sensing Ltd.* (**Baker**); £350k from Eastman (**Clarke**); £34k from *UCB Celltech* (**Michel**); £145k from *Sunamp* (**Pulham**); £62k from *Integrated Graphene* (**Schaub**) resulting in further funding of £124k from SFC and Innovate UK/£2.3M to *Integrated Graphene* from the Faraday Battery Challenge; £25k from *GSK* (**Thomas**); £108k from *GSK* (**Wright**/**Clarke**); £300k from *Cynora* (**Zysman-Colman**). *ZEMFuels* was formed as a spin-out company (**Irvine**) to commercialize technology developed through IAA-funded research.
- A policy of providing matched funds for externally funded PhD studentships has helped generate 112 industrially-linked PhD studentships. This provides an effective mechanism for solving industrial problems and seeding long-lasting collaborations, such as those between **Camp**/*Infineum*, **Pulham**/*Sunamp* (both now ICSs), and **Uhrin**/*Glycomar*.
- Sabbatical leave for impact development has cemented successful collaborations: **Schaub** with *Integrated Graphene*; **Love** with a GCRF consortium on reclaiming gold from urban mining; **Heal** with the *Defra Air Quality Expert Group*; and **Morris** with *MOFGen* (ICS on commercialisation of porous materials). RS Industrial Fellowships also enable focus on impact (**Clarke** with *Dr Reddy's*, **Webb** with *Sasol*, and **Wright** with *Johnson Matthey*).
- Increased training opportunities for PDRA and PhDs communities, including an annual lecture series on commercial awareness, entrepreneurism, and research commercialisation.
- Since 2014, a total of 47 patent applications were filed by **UoE**/**UStA**, with EaStCHEM staff named as inventors, to protect IP that may generate impact.

Objective (3) Facilitating interactions with research users

The following illustrates our mechanisms to facilitate interactions with research users.

- We have developed long-term strategic partnerships resulting in an EPSRC Prosperity Partnership with *BP* ("Preventing Surface Degradation in Demanding Environments" **Camp**/**Pulham**) and *Rolls Royce* in *GENESIS* at the **Eden Campus**.
- Our world-class facilities attract SMEs and large national/international companies. Investment in dedicated facilities management has ensured provision of a high-quality service, which has provided a revenue of £1.4M, seeded collaborations, and generated impact (Section 3).
- We ring-fence on-site lab space and facility access to SMEs and spin-outs, which has proved particularly valuable at the early stage of their existence. For example, spin-out successes *Invizius*, *MOFGen*, and *Gemini Therapeutics*, highlighted as ICSs, were all supported in this way. In addition, *Edinburgh Molecular Imaging*, *Red-T/Invinity Energy Systems*, *The Falcon Project*, *LERC*, *ZEMFuels*, and *Drochaid* have all co-located within EaStCHEM and have worked closely with our researchers.
- Year-long student placements in industry, as part of undergraduate degree programmes, seed new contacts and have provided valuable support to our spin-outs and existing partners (308 placements with 81 companies since 2014). At PhD level, industrial placements are embedded in the CRITICAT, EaSICAT, and OPTIMA programmes.

1f. Open research and research integrity/ethics

Creating an open research environment: EaStCHEM is committed to ensuring the widest access to its research through providing Open Access and Open Data to published outputs. Building upon institutional support (**UStA**/**UoE** IES, Section 2), we have provided dedicated administrative resource and clear mechanisms for open research to minimise additional work-load for academic staff. As a result, our Open Access compliance rate is 92% (based on 1953 outputs published since 1st April 2016). For Open Data, we have developed discipline-specific guidance notes on what constitutes data, what makes good metadata, and what compliance means for chemistry outputs, particularly those resulting from research funded by UKRI or the EU. To help staff achieve compliance, these policies and mechanisms were communicated to staff through a series of workshops, and with guidance published online. Underpinning data for over 600 datasets has been published in the EaStCHEM research repository (PURE) since 1st April 2016.

Research integrity/ethics: EaStCHEM's approach to research integrity and ethics follows institutional best practice (**UStA**/**UoE** IES, Section 2), with clear and robust procedures to report and investigate allegations of scientific misconduct. To ensure that EaStCHEM's high expectations for research integrity and ethics standards are met, we have developed a code of practice based closely on the policies and procedures of the *UK Research Integrity Office*. These define the principles and expectations for research conduct, and ensure that EaStCHEM research is subject to the appropriate ethical, legal, and professional standards. All staff, PDRAs and postgraduate students undertake mandatory online research integrity and ethics training modules that support and foster best practice.

1g. Future plans

Over the next ten years we will build on the EaStCHEM synergistic partnership, with our strategy designed to: (**1**) address significant challenges in each of our research themes; (**2**) to invest in people to sustain momentum and improve our diversity; (**3**) maintain our trajectory and focus upon impact generation; and (**4**) maintain and improve our pooled infrastructure.

Research: our five research themes are well positioned to address global challenges and showcase interdisciplinarity through our fundamental and applied research. In **T-CBI**, we will take chemistry into the operating theatre with non-invasive imaging technologies for medical diagnostics and interventions, and develop new computational technologies to accelerate preclinical drug development. In **T-CS** we will develop and improve new catalytic reactions that use earth-abundant materials to maximise resource use and minimise waste across industrial processes. In **T-FM** we will design new materials, making increasing use of predictive computational and data-driven approaches, for applications including energy conversion and storage, gas separations, and quantum computing. In **T-SCCD** we will follow chemical reactions and processes in real time and on rapid timescales to advance insight into fundamental processes covering the whole of chemistry. In **T-EES** we will continue to monitor key parts of the environment (air quality, peatland), and develop techniques for recycling/urban mining of polymers and metals. We will demonstrate the potential of hydrogen as an energy vector in the transportation sector via the *Hydrogen Accelerator*.

People: a projected 15 retirements over the next decade, together with the continuation of our strategy of sustainable growth in staff numbers, will provide the opportunity for future appointments at all levels. This will include a minimum of two named Chair positions (**Crum Brown**, **Industrial Chemistry**) to provide leadership at senior level. Building on our flagship **Christina Miller** and **Ettie Steele** Fellowships, which have resulted in the development of talented women ECRs into future research leaders (Section 2), we will target recruitment from under-represented groups to achieve a balance that better reflects the diversity of UK society. We will broaden our mentorship schemes to enable ECRs/PDRAs to benefit from the experience of peers and senior colleagues across EaStCHEM, enhance institutional links, and initiate new collaborations.

Impact generation: we will build on our current momentum to further enhance staff engagement with industry and policy makers in order to translate research into impact leading to major contributions to healthcare, energy, sustainability, and climate change. This will be achieved by strengthening the Impact Team by the appointment of a permanent full-time EaStCHEM Impact Coordinator and the establishment of an Impact Strategy Board with external representation. We

will continue to appoint staff who have the potential to deliver impact, e.g. in 2021 we will fill the vacant **Chair of Industrial Chemistry** and appoint **Agnew** (former Chief Technologist at *Rolls-Royce*) to a personal chair.

Infrastructure: significant new builds will accommodate chemical research at the biological/medical interface. At **UStA** a £15M refurbishment (estimated completion August 2022) will replace the building damaged by fire in February 2019, while at **UoE** a £39M investment will develop new interdisciplinary laboratories within **The Edinburgh BioQuarter**, Scotland's leading hospital campus (Section 3c). We will continue to maintain, renew, and improve our pooled infrastructure to ensure that EaStCHEM staff will have access to state-of-the-art facilities.

2. People

2a. Staffing strategy

Across EaStCHEM we have appointed talented researchers who add excellence to our research strengths and share our commitment to an environment that is supportive to all.

Strategic appointments: as noted in Section 1b, newly appointed staff have strengthened research and impact activity across our research themes, enhanced interdiscipinary links (Section 1d), and improved our diversity. We welcomed 29 new academic staff, spanning independent ECR fellowships (13), lectureships (9), readerships (3) and chairs (4), increasing academic staff numbers to 88.3 FTE from 80.6 submitted to REF2014.

Enhancing gender balance: following an analysis of ECR appointments during REF2014 (Fig. 8), it was clear that EaStCHEM's gender balance would remain poor unless affirmative action was taken. As a consequence, we implemented our **Christina Miller** (**CMF**) and **Ettie Steele** (**ESF**) Fellowship schemes, which are targeted at under-represented groups who are traditionally less likely to follow an academic career and may lack the confidence to apply directly to conventional fellowships. These schemes helped to achieve gender balance for ECRs recruited since 2014 (Fig. 8), and increased the overall proportion of female staff to 23% (from 16% submitted to REF2014). The continuation of these schemes shows our future commitment to deliver targeted recruitment from under-represented groups, and to enable EaStCHEM to approach a gender and diversity balance that better reflects society. In addition, we have incorporated best-practice ED&I processes for recruitment across EaStCHEM, including: (**1**) scrutiny of the language used in adverts to encourage applicants from all groups; (**2**) unconscious-bias training for all panel members; (**3**) gender-inclusive appointment panels; and (**4**) targeted advertising to under-represented groups.

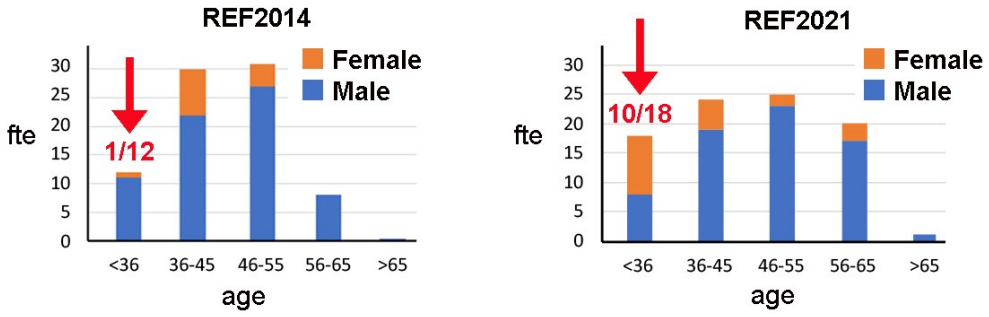

Fig. 8. *The REF2014 and REF2021 staff/age profiles showing the correction of the gender imbalance for ECRs during this assessment period.*

2b. Staff development and support

EaStCHEM prides itself on providing a highly supportive environment for career development, and nurturing talent at all levels to fulfil their research and impact potentials.

Direct support is provided by the allocation of studentships from both internal and external funding, such as the EPSRC Doctoral Training Partnership (DTP), by a transparent and fair process overseen by Studentship Allocation Committees. Strategic prioritisation is given to newly appointed staff and projects that have high potential to generate impact via industrial engagement.

Support for new staff: induction includes tailored programmes relevant to gaining skills in research, impact, and teaching, which contain school-specific, university-wide and EaStCHEM training components. Each new staff member is allocated an academic mentor to provide support and guidance during the transitional period of setting up a research group and achieving a successful independent portfolio of grants and outputs. Mentors and senior colleagues also provide informal peer review of grant applications.

Support across career progression: staff have annual performance and development reviews. Training courses are offered for the development of vital academic skills such as grant writing, supervision of PhD students, and leadership. Interview practice is provided for fellowships (e.g. UKRI Future Leaders) and major grant applications (ERC, UKRI), which has contributed to successful awards (Section 3). The expectation is that all appointed research-active staff have the potential to achieve the status of Professor or Reader, consistent with an increasing proportion of staff of age >45 who are Professors (65%). During the assessment period there were **19** promotions to Personal Chair (**Ashbrook**, **Baddeley**, **Camp**, **Colin Campbell**, **Campopiano**, **Clarke**, **Cockroft**, **Goss**, **Heal**, **Hulme**, **Jones**, **Lawrence**, **Love**, **Morrison**, **Robertson**, **Seery**, **Shaver**, **Westwood**, **Zysman-Colman**) and **3** promotions to Reader (**Aitken**, **Alexander**, **Thomas**).

The following staff have left to take up prestigious external positions that reflect positively upon their career development at EaStCHEM.

- **Arnold** to Chemical Sciences Division Director at the Lawrence Berkeley National Labs.
- **Cazin** to Professor of Chemistry, Ghent University.
- **Duarte** to Associate Professor of Chemistry, Oxford University.
- **Kamer** (deceased) to Professor of Homogeneous Catalysis, LIKAT, Rostock.
- **Moggach** to Professor of Structural Chemistry, University of Western Australia.
- **Naismith** to Director of the Rosalind Franklin Institute.
- **Shaver** to Professor of Polymer Science, University of Manchester.
- **Vogt** to Professor of Chemical Engineering, Dortmund Technical University.

Time for research and impact: the EaStCHEM Board prioritises staff time for engagement in research and impact. Teaching commitments have been reduced significantly by employing **9** teaching-focussed lecturers whose remit is to professionalise and update our undergraduate programmes. Newly implemented workload models ensure that time to concentrate on research and impact is correctly balanced against the time commitments of teaching and administration. In particular, ECRs have reduced teaching loads to allow them to focus on building their research groups. Further support for research and impact comes from dedicated teams of administrative, technical, and computing staff. We have increased our investment in expert facility managers (up to 20 from 14 at REF2014) to professionalise these services and provide research time for staff.

Research or impact sabbaticals: with recognition of their importance for the development of research programmes and impact, staff with >4 years of service are eligible to apply for a sabbatical period of up to 12 months. Fifteen research sabbaticals were taken, most of which involved extended visits abroad including: *Queens University*, Canada (**Baddeley**); *Technical University of Berlin* (**Buehl**); *Biofrontiers Institute in Boulder*, USA (**Colin Campbell**); *University of Nagoya*, Japan (**Eleanor Campbell**, **Shaver**); *University of Campinas*, Brazil (**O'Hagan**); and *Northwestern University*, USA (**Philp**). As an example of the success gained from sabbatical leave, **Baddeley**'s resulting collaboration with Crudden (Queens University) demonstrated the direct formation of self-assembled N-heterocyclic carbene films on gold and their application in biosensing (*Nature Commun.* **2016**). This led to funding from UKRI (EP/S027270/1, £500k) with Queens as a research partner. Impact sabbaticals were also initiated to stimulate collaborations with research users resulting in significant funding and impact (e.g. **Schaub**/*Integrated Graphene*, Section 1d).

Recognising research and impact performance: in addition to promotions, excellence in research and impact is rewarded by nominations for prizes and awards resulting in great success during this assessment period (40 in total – see Section 4f).

2c. Equality, diversity, and inclusion

Equality, diversity, and inclusion (ED&I) are core EaStCHEM values promoted by our active ED&I committees, the chairs of which sit on each School's management group. These committees draw membership from undergraduates, postgraduates, research/teaching staff, and professional services staff to ensure that a diversity of voices are represented. Major infrastructure initiatives in this period include the establishment of gender-neutral toilets, improved disabled access, as well as communal social space and dedicated wellbeing and multi-faith prayer rooms (£1.0M; Section 3c). Training has been provided in mental health awareness, the identification and prevention of bullying and harassment, and resilience training (of particular importance with disruption due to COVID-19) to help ensure that EaStCHEM provides an inclusive and supportive environment to ***all*** staff and students. We celebrate ED&I through informal social events including Ada Lovelace Day and International Evenings.

Supporting under-represented groups: Four BAME staff have been appointed as ECRs and future appointments will be facilitated by more targeted use of the **CMF**/**ESF** schemes to encourage applications from under-represented groups. We have prioritised the development of our ED&I policies to provide a fair and inclusive environment for all staff/students with protected characteristics, resulting in increased access and support for disabled staff/students.

Supporting gender equality: our achievements in promoting gender equality were recognised by *Athena Swan Silver* (**UoE**) and *Bronze* (**UStA**) awards during the assessment period. We are particularly proud of our pioneering **CMF** and **ESF** schemes, which have helped the following exceptional female researchers transition to independence (Section 2a).

- **Garden** from PDRA (Imperial College) to CMF (2016-17) to British Ramsay Memorial Trust Fellowship (2017-20) to UKRI Future Leaders Fellowship (2020-).
- **Jarvis** from a Marie Curie Individual Fellowship (**UStA**) to CMF (2017-19) to UKRI Future Leaders Fellowship (2019-).
- **Payne** from PDRA (**UStA**) to ESF (2018-).
- **Hobday** from PDRA (Bath) to CMF (2018-2020) to Chancellor's Fellowship (2020-).
- **Mey** from PDRA (**UoE**) to CMF (2019-2020) to Chancellor's Fellowship (2020-).

Further evidence for the success of our "*appoint and nurture*" strategy is shown by **Bell** who transitioned from a 3-year NERC Soil Security Fellowship to a 5-year NERC Independent Fellowship, and **Duarte** who transitioned from Chancellor's Fellow to Associate Professor of Chemistry (Oxford). As a consequence of this strong support for talented female ECRs, gender balance has been achieved for EaStCHEM ECRs (Fig. 8). While these are positive steps, we recognise that it is essential for support for female staff to be sustained throughout their careers, and so the following initiatives were implemented.

- Flexible paternity/maternity arrangements including opportunities for phased return to work with options for alternative working arrangements.
- All formal meetings and academic symposia are scheduled within core hours.
- All non-professorial staff are considered annually for promotion.

In addition to exceptional support for female ECRs, the following is evidence that women thrive throughout their careers within EaStCHEM.

- Chair promotions (**Ashbrook**, 2013; **Goss**, 2018; **Hulme**, 2018; **Jones**, 2015; **Morrison**, 2019) have increased the number of female professors to 7 (from 3 submitted in REF2014).
- **Arnold** elected RS Fellow (2016) and awarded OBE (2018).
- **Ashbrook** (2016) and **Goss** (2020) elected RSE Fellows.
- **Ashbrook** presented with a Wolfson Merit Award (2015).
- **Cazin** awarded Sir Thomas Makdougall Brisbane medal of the RSE (2014).
- **Eleanor Campbell** elected President of the Faraday Division of the RSC (2015-2018) and Member of *Academia Europaea* (2018).
- **Hulme** elected President of the RSC Perkin Division (2017-2020).
- **Slawin** recognised in 2018 by the *Cambridge Crystallographic Data Centre* (CCDC) as the woman who has contributed the most XRD structures (3350!).

- The award of prizes to **Arnold** (RSE Lord Kelvin Medal, 2017), **Ashbrook** (RSC Corday-Morgan, 2015), **Bell** (RSC Joseph Black Award, 2017), **Eleanor Campbell** (Ubbelohde Prize, British Carbon Group, 2016), **Garden** (Macro Group Young Investigators Award, 2019; *L'Oreal-UNESCO* Women in Science Fellowship, 2019), and **Hobday** (CCDC Chemical Crystallography Prize for Younger Scientists, 2018; Durward Cruickshank Young Crystallographers' Prize, 2018).
- **Arnold** and **Ashbrook** provided national leadership on the issue of promoting women in chemistry (Section 4d) as recognised by *Suffrage Science Awards*.

ED&I in REF preparations: ED&I was carefully considered during the preparation of EaStCHEM's REF2021 submission. All staff involved in developing the submission and assessing outputs completed a specific training course on ED&I, and we have followed strictly policies and processes set out in our institutional codes of practice. Inclusion in the output portfolio was based solely on quality as determined by a gender-inclusive panel of staff members, all of whom had taken unconscious-bias training. Of the 221 submitted outputs, 63 (29%) contain a female staff member as author, which is greater than the proportion of female staff (22%).

2d. Early-career researchers

During the assessment period, EaStCHEM selected, via rigorous appointment processes, an excellent cohort of ECRs including 3 lecturers (**Cumby**, **Horrocks**, **Szabla**) and 18 who succeeded in obtaining competitively awarded fellowships both internally from the **UoE**'s tenure-track Chancellor's Fellowship (**Clarke**, **Duarte**, **Erastova**) or **CMF**/**ESF** (**Garden**, **Hobday**, **Jarvis**, **Mey** and **Payne**) schemes, and externally from the RSE/BP Trust Fellowship (**Johansson**), Leverhulme Early Career Fellowship (**Kumar**, **Lancefield**, **Pal**, **Taylor**), NERC Soil Security Fellowship (**Bell**), RS URF (**Ewen Campbell**, **Johnston**), UKRI Innovation Fellowship (**Yue**), and UKRI Early Career Fellowship (**Gibbs**) schemes.

Appointment and progression: all ECRs, including fellows, are appointed with the firm expectation that their research performance will merit retention on completion of their probationary period or fellowship. As such, they are immediately viewed as highly valued and fully independent members of the academic staff. Potential applicants to fellowships are interviewed to ensure they provide a good strategic fit to EaStCHEM's research, and they are committed to contributing towards its collegiate environment. Once approved, help to achieve fellowships includes: (**1**) a strong letter of support that commits to generous start-up funds including studentships; (**2**) mentorship and feedback on draft proposals; and (**3**) mock interview practice with experienced staff. There is an expectation that all ECRs and fellows progress to the level of Reader or Professor within 10-15 years of appointment (excluding career breaks). However, it is recognised that it can take time to excel at group leadership, generation of impact, teaching, knowledge exchange, and outreach. Support is provided from both an academic mentor and an established laboratory host, and feedback is given on draft grant proposals. All ECRs and fellows are eligible to apply for competitive internal resources such as DTP/School or University funded studentships, and funding for conference attendance and equipment. A reduced teaching/administration load, particularly during the two-year period following appointment, allows for rapid establishment of research activity. Progress is reviewed each year via *Performance and Development Review* (P&DR) and, for fellows, a full review after three years ensures that they are on track for an open-ended lectureship appointment.

Nurturing success: a project jointly funded by EaStCHEM and the *Wellcome Trust's Institutional Strategic Support Fund* sought to understand why only a relatively small number of academics are successful at leading large interdisciplinary proposals and building research clusters. Diversity issues relating to the award of large UKRI grants were also investigated by a collaboration between physical and social scientists funded by the EPSRC grant "*Evidence Base: Growing the Big Grant Club*" (**Arnold**). In both studies it was found that PIs develop the necessary confidence and entrepreneurial skills early in their career. Consequently, all ECR staff are given specific training in leadership and the networking skills required to develop large grants and fellowship applications.

- Our successful "*appoint and nurture*" strategy is demonstrated by the progression of **Garden** and **Jarvis** to UKRI Future Leader Fellowships, **Bell** to a NERC Independent Researcher

Fellowship, and **Hobday** and **Mey** to Chancellor's Fellowships. In addition, the following ECRs have achieved permanent academic positions: **Duarte** (Associate Professor, *Oxford*); **Johansson** (Lecturer); **Pal** (Lecturer, *IIT Jammu*); and **Taylor** (Lecturer, *Bath*).

- ECR fellows appointed prior to this REF period have also successfully transitioned to permanent positions: **Bode** (Lecturer from EaStCHEM Fellow); **Cowley** (Senior Lecturer from Chancellor's Fellowship); **Kay** (Lecturer from RSE Fellow); **Kirrander** (Senior Lecturer from Chancellor's Fellowship); **Lilienkampf** (Lecturer from University Fellow); **Michel** (Senior Lecturer from RS URF); **Nudelman** (Senior Lecturer from Chancellor's Fellow); **Shaver** (Chair of Materials, *Manchester* from Chancellor's Fellowship); **Thomas** (Reader from RS/URF extended); and **Zysman-Colman** (Chair from EaStCHEM Fellow).

2e. Postdoctoral reseach associates

PDRAs are valued members of staff who contribute greatly to the success of EaStCHEM, but in the past, they were not offered the same opportunities for professional development as PGR students. As a result, staff follow the *Vitae Concordat* to support the career development of researchers, and we have developed the following initiatives.

- To promote networking and collaboration, and develop research and leadership skills, the annual EaStCHEM Conference for Early Career Researchers (ECECR) was established in 2016. Hosting alternates between **UoE**/**UStA**, and there is an annual attendance of >100 PDRAs and ECRs.
- PDRA Committees promote social, cultural, and scientific events.
- There is PDRA representation on Safety, ED&I and Staff Committees.
- Members of academic staff act as Champions to represent PDRA interests.
- Training courses to improve academic skills (such as writing grant and fellowship proposals, networking and leadership) are provided by EaStCHEM and University units.
- Career development advice is provided by supervisors at annual P&DR meetings.

2f. Postgraduate research (PGR) students

Number of students and funding sources: PGR students are central to our research activities in EaStCHEM. During the assessment period, we awarded 526 doctoral degrees, with most proceeding on to post-doctoral study or industrial jobs in chemistry related disciplines. Both Schools have invested in the collaborative *EaStCHEM PhD Studentships Scheme* (£900k investment) involving PI co-supervision and research time (at least 12 months) at both **UStA** and **UoE**. A variety of PhD studentship opportunities have been offered as follows.

- EaStCHEM-based training programmes that combine high quality research with skills development training such as *OPTIMA* (Optical Medical Imaging), *CRITICAT* (Critical Resource Catalysis) and *EaSICAT* (East of Scotland Industrial Catalysis).
- Training centres including *EaStBIO BBSRC Training Partnership*, *Industrial Biotechnology Innovation Centre* (*IBioIC*)-CTP, *Soft Matter and Functional Interfaces* (*SOFI*) CDT, and *NERC Edinburgh Earth, Ecology and Environment* DTP.
- EPSRC/DTG funds combined with EaStCHEM investment.
- China Scholarships Council, with whom strong links have been developed (47 studentships).
- Marie-Curie ITN networks (*SubiCAT*, *PhotoReact*, and *TADFLife*).
- Industry (112 studentships).

Monitoring and assessment: all postgraduate research students are members of the EaStCHEM Graduate School, with progression monitored by individual Schools. The Graduate School Committees, led by **Westwood**/**Kilian** and **Nudelman**, oversee supervision and training quality, and ensure effective milestone monitoring across all programmes. To emphasise cohesiveness within EaStCHEM, **UStA** and **UoE** have amended their regulations to allow staff from either partner to act as internal PhD examiners. Key events on the path to a PhD are an assessed written report, viva, and presentation for all students on a yearly basis throughout their PhD studies, plus a departmental research presentation at an annual Postgraduate Symposium. Progress is assessed by a thesis committee for each student, consisting of their primary and secondary supervisors and an independent academic. Assessment is recorded by written reports

through an on-line electronic system (MMS, **UStA**; EUCLID, **UoE**), with students given access to feedback. The 4-year completion rate for PhD students across EaStCHEM is >90%.

Support for PhD students: the EaStCHEM Graduate School, working with the *Institute for Academic Development* (**IAD**) and *Centre for Academic, Professional and Organisational Development* (**CAPOD**), provides core PhD training courses and events that integrate transferable and scientific skills. In addition to mandatory training on research integrity and ethics, joint EaStCHEM Graduate School courses include popular programmes on project management, how to write a thesis, and the preparation of papers for academic journals. In addition, EaStCHEM provides vibrant and inclusive social activities via the following organisations.

- *Chemunity*: a scheme to build social networks to help mental health and well-being.
- Long-established and very active *Chemical Societies* that organise frequent social events (such as Annual Balls, Burns Night celebrations, Quiz Nights) as well as academic and industrial lectures.
- *International Societies* that organise social events for all PhD students.

Not only have these initiatives helped build inclusive communities, but also they have provided much needed support during the COVID-19 pandemic.

3. Income, infrastructure, and facilities

EaStCHEM has spent >£113M of research funding in the REF period including >£9M from industry. To underpin our research strategy (Section 1), we have enhanced our infrastructure and established further shared cutting-edge facilities to: (**1**) enable world-class research; (**2**) professionalise and expand our technical support base; (**3**) support a safe working environment for all researchers; and (**4**) promote facility use to external users to raise income and further impact activities.

3a. Research income

Major awards (see Section 4a for international consortia funding): initiatives to enhance funding include targeted workshops for ERC applications and practice interviews for short-listed applicants for ERC Starter and Consolidator Grants. This helped to achieve a significant increase in ***EU funding*** (from £2.7M p.a./REF2014 to £3.7M p.a./REF2021, total £26M), including 6 ERC Advanced Investigator Grants (**Arnold**, **Attfield**, **Bradley**, **Lloyd-Jones**, **Morris**, **Naismith**), 3 Consolidator Grants (**Goss**, **Ashbrook**, **Ingleson**), and 4 Starter Grants (**Cowley**, **Lawrence**, **Cockroft**, **Michel**). Rigorous interview practice also helped to achieve major ***UKRI*** platform grants: "Putting the squeeze on molecule-based magnets" (**Brechin**, EPSRC, £1.3M); "Exploring electronic materials under extreme conditions" (**Attfield**, EPSRC, £1M); Critical Mass grant "Emergent Nanomaterials" (**Irvine**, EPSRC, £1.6M); and IRC grant "Proteus" (**Bradley**/**Megia-Fernandez**, EPSRC, £4.3M). Similarly, it helped staff to secure the following Fellowship grants: "Assembly, disassembly, reassembly - new routes to extended structures and their impact" (**Morris**, EPSRC, £1.3M); "Artificial metalloenzymes as evolvable catalysts for selective chemical synthesis" (**Jarvis**, UKRI Future Leaders, £1.4M); "Next generation advanced materials: structure-property relationships" (**Gibbs**, EPSRC, £1.2M); and "Molecular, microbial and enzymatic synergies and their significance to peatland condition" (**Bell**, NERC, £700k). Focused workshops on writing ***GCRF/ISCF*** proposals helped to achieve the following grants: "NEXGENNA Faraday Challenge Award" (ISCF**, Irvine**/**Armstrong**, £12M); "Chemical recycling of electronic waste for sustainable livelihoods and material consumption in India" (GCRF, **Love**, £400k); and "Equitable access to Quality Antibiotic Therapies in Africa" (GCRF, **Florence**, £900k).

Industry funding: industry is a significant contributor to EaStCHEM research funding with the following major grants awarded during the assessment period: *Eastman Chemicals* (£1.5M); *LERC* (£1.1M); *Evonik* (£770k); *AGT Management* (£720k); *Castrol* (£700k); *AWE* (£480k); *Cynora* (£300k); *BP* (£277k); and *Infineum* (£300k). Smaller grants to support PhD studentships (£20k-£108k) were obtained from *AstraZeneca* (16), *GlaxoSmithKline* (14), *Syngenta* (5), *Johnson Matthey* (3), *Sasol* (3), *Axis-Shield* (2), *Pfizer* (2), and *UCB Celltech* (2), with a further 35 partners providing support for a single PhD studentship. Smaller studentship grants seeded research that

evolved to larger collaborations, such as that between *AstraZeneca* and **Thomas** on Group 13 catalysts.

3b. Organisational infrastructure supporting research and impact

Professionalising facilities: a key benefit of EaStCHEM is the pooling of research equipment that ensures cutting-edge facilities are available to all researchers at each institution. These state-of-the art facilities are led by exceptional scientists (**Ashbrook**, **Bode**, **Clarke**, **Irvine**, **Parsons**, **Slawin**, **Uhrin**), and operated by experienced facility managers and technicians. Salary contributions from each institution are made to staff, and technical support is provided for joint ventures such as *The Scottish High Field NMR Centre*. The provision of expert facility managers across NMR (4), MS (3), XRD (2), ICP elemental analysis (1), surface science (1), electron microscopy (1), high-performance computing (0.4), and fermentation (1) ensures the smooth running of facilities, and unhindered access to internal and external users. Research is also supported by efficient mechanical, IT, electrical and glassblowing workshops. Complementarity is maintained over the two institutions with, for example, **UoE** hosting high-field NMR instruments for liquid samples, whereas **UStA** specialises in solid-state NMR and EPR.

Supporting a safe working environment: EaStCHEM's top priority is to ensure a safe working environment for all researchers. This has prompted the recruitment of a dedicated Health and Safety Manager (**Easdale**) who has previous experience in a similar role in the chemical industry. This appointment has had a very positive effect on the working practices at **UoE**, and therefore, a similar dedicated position has been created at **UStA**, with the new appointment (**Jones**) starting in Feb 2021. In response to the devastating fire in the **Biomolecular Sciences** (**BMS**) building (February 2019), bespoke automated metal containers have been designed to prevent the spread of fire when using plastic isopropanol/KOH wash-baths. An additional strategy to prevent fires provided investment (£250k) for a solvent purification laboratory, which enables safe access to dry solvents for all research groups. In addition, the EaStCHEM Board has devised a detailed Business Continuity Plan which includes dealing with unforeseen events that can disrupt research. An example is provided by the close sharing of detailed plans and best practice for resuming research activity after the lockdown caused by the COVID-19 pandemic, resulting in both Schools being among the first to reopen for research at each University.

Use of infrastructure, facilities and expertise in impact activities: the generation of impact is a key driver for providing access to EaStCHEM facilities for industrial and other external users. There has been a significant increase in external revenue to £1.4M across our facilities during this assessment period, with a notable expansion of NMR services (from £7k in 2014 to £58k in 2020, £249k in total). Impact generated directly from within EaStCHEM services and facilities during the REF period includes the following.

- The development of novel MS techniques to characterise and quantify *Bioven*'s promising lung cancer vaccine EGF-PTI, in order to confirm batch purity and consistency before its US/EU Phase III trials (MS Facility Manager **Mackay**).
- MS 3D imaging of cell cultures was used by *AstraZeneca* for screening the distribution of drug candidates in cells, thus reducing the need for animal models (**Mackay**). *AstraZeneca*'s Head of Imaging reports that data from EaStCHEM, "*combining high spatial resolution with the highest spectral resolution*", was "*crucial for decision making*" in the progress of seven internal projects.
- In collaboration with *The Scotch Whisky Research Institute*, the complexity of Scotland's favourite tipple and highest-value export has been investigated using high-resolution MS and NMR, leading to novel methods of establishing provenance and authenticity (**Uhrin**, *J. Am. Soc. Mass Spectrom.* **2017**, *Food Chem.* **2019**).

3c. Infrastructure investment

EaStCHEM has been the beneficiary of major governmental and institutional investment in infrastructure to enhance its research environment.

City Deals: a significant multimillion-pound investment by government (£30M as part of the *Tay Cities Deal*) and industry (11 companies, £8M) has resulted in the *Scottish Centre for Clean Energy Storage and Conversion and Enterprise Hub* on the **Eden Campus** with EaStCHEM a

major beneficiary (**Irvine**, **Webb**, **Goss**, **Schaub**). The *Edinburgh and South-East Scotland City Deal* on Data-Driven Innovations has helped stimulate projects on the application of machine learning to crystallography (**Cumby**/**Hobday**) and polymer design (**McKeown**), and provided collaborations with the *Bayes Centre* for data science (**Michel**/**Mey**).

Investment in buildings: institutional investment facilitated hosting of: (**1**) the DECC-funded *Pyrochemical Research Laboratory* (PRL, **Mount**, £1M), which is an open access facility affiliated to the *National Nuclear Laboratory*, providing integrated pyrochemical reprocessing of nuclear fuel; and (**2**) the building of the *Electron Microscopy and Light Element Analysis Centre* (£2.4M) (Section 3d). The fire in the **BMS** building displaced seven research groups, which were rehoused and operational within one month thanks to efficient space management and the goodwill of EaStCHEM colleagues. A rapid renovation (£2M) to replace synthetic chemistry laboratories lost in the fire (30 fume cupboards) was completed in June 2020. A major refurbishment of the **BMS** building (£15M), due for completion in August 2022, will provide significant workspace at the Chemistry-Biology interface (**O'Hagan**, **Goss**). The building of new laboratories within **The Edinburgh BioQuarter** at Little France, Scotland's leading hospital campus, has been confirmed with an institutional investment of £39M. This interdisciplinary hub will allow the research cluster led by **Bradley**, which develops chemical processes for medical imaging and *in-vitro* drug activation, to benefit from major future UKRI investment at the medical science/physical science interface (Section 4).

General refurbishment: additional institutional investment from **UoE**/**UStA** (£1.35M) and RS funding (£250k) has allowed laboratories and offices to be refurbished for newly appointed/current staff. General building refurbishment (£2M) has upgraded lecture theatres, disability access, a first-aid room, WiFi provision, and a loading bay, and provided a modern social space used by all **UoE**-based students and staff. Training of Year 4 **UoE** undergraduate students in research techniques (**Daff**) has benefited from a bespoke new laboratory (£220k) with equipment provided by a donation from *Afton Chemicals* (£85k).

Environmental sustainability: institutional investment from **UoE**/**UStA** (£1.5M) has been used to reduce the cost and environmental impact of research by upgrading fume cupboards and ventilation (saving over £100k in energy costs and 500 tons of CO_2 emissions per year). The provision of chillers for rotary evaporators and air condensers for refluxing reactions is estimated to save 600 m^3 of water annually. Replacement of a rotating anode for XPS (**Baddeley**, £129k), and an upgrade to single crystal X-ray analysis (**Slawin**, £111k) have also been possible through energy efficiency savings. The investment of helium recovery units for NMR and MS magnets at both **UoE** and **UStA** (£100k) will pay for itself in 8 years, and guarantees an uninterrupted supply during regular world-wide shortages, thus eliminating potential damage to essential equipment.

3d. Improvements to provision of facilities supporting research and impact

NMR: EaStCHEM provided leadership to the *Scottish NMR Users Group* (SNUG) that successfully bid to EPSRC to establish the *Scottish High Field NMR Centre* (**Uhrin**/**Ashbrook**, £1.4M). The Centre operates an 800 MHz Bruker spectrometer, accessible to EaStCHEM users and Scottish researchers, across physical and biological sciences. Supported by *ScotCHEM* and the *Scottish Universities Life Sciences Alliance* (£69k), the Centre distributes competitive grants to facilitate the preparation of biomolecules (often isotopically labelled) for structural biology studies. Other NMR facility investments (£1.5M) include the purchase of an AVIII-HD-700 instrument and upgrades (including cryoprobes and console) to existing spectrometers.

MS: BBSRC funded the purchase of a state-of-the-art 12T/SolariX/2XR/FT ion cyclotron resonance MS (**Campopiano**/**Clarke**, £750k) which enhances and complements EaStCHEM's already impressive MS suite.

Diffraction: single-crystal X-ray diffraction (XRD) facilities were augmented by the EPSRC-funded purchase of a diffractometer (**Parsons**, £560k), specifically to maintain EaStCHEM's world-leading research on high-pressure XRD. EPSRC core equipment bids led to upgraded powder XRD facilities for materials characterisation (**Payne**, **Kirk**, £800k).

Materials characterisation: the *Centre for Science at Extreme Conditions* (CSEC) provides EaStCHEM researchers access to expertise and wide-ranging facilities to study the structure and

properties of matter (e.g. XRD, magnetism, and calorimetry) when subjected to extremes of pressure and temperature. In addition to upgraded XRD facilities (as above), EPSRC funded a Physical Properties Measurement System (PPMS) (**Attfield**, £600k).

EPR: institutional investment and BBSRC funded a cryogen-free cooler and Arbitrary Waveform EPR (**Bode**, £350k).

Microscopy: the *Electron Microscopy and Light Element Analysis* Centre (**Irvine**, £7.9M total investment) has been enhanced by EPSRC funding (£1.5M) for an electron probe microanalyser (EPMA), a separate soft X-ray emission spectrometer (SXES) system, and a confocal Raman microscope. For the characterisation of soft matter, a cryo-SEM with focussed ion beam has been funded by EPSRC (**Nudelman**, £1.3M).

High performance computing (HPC) facilities: access to world-leading HPC facilities, hosted by the **Edinburgh Parallel Computing Centre** and the UK's materials and molecular modelling hub, underpins research by **Buehl**, **Erastova, Hobday**, **Mey**, **Mitchell**, and **Morrison** (EPSRC UKCP consortium, £470k). Computing facilities across the Science Schools at **UStA** have been upgraded with £1.3M investment.

3e. In-kind use of facilities and donations

Significant in-kind contributions to EaStCHEM facilities include bespoke ultra-high vacuum equipment (Fig. 9, acquisition value £800k) from the Maier laboratory at the *University of Basel*, to continue **Ewen Campbell**'s URF-funded research into astrochemical fullerene formation (*Nature*, **2015**). The **School of Physics** donated a 300 MHz solid-state NMR spectrometer (acquisition value £300k). Links to the **Organic Semiconductor Centre** allow EaStCHEM researchers access to the newly refurbished £2M clean room facility.

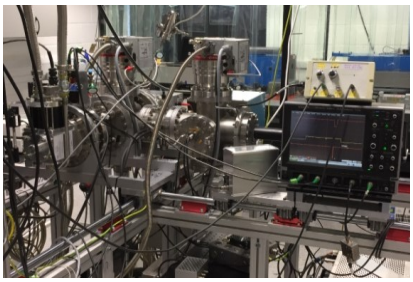

Fig. 9. *A gift from Basel: the astrochemical laboratory.*

3f. Use of major facilities

The extensive use of major facilities by EaStCHEM staff is indicated by the 240 outputs published since 2014 that are co-authored with researchers at a UK/international major facility.

UKRI: EaStCHEM researchers (e.g. **Attfield**, **Gibbs**, **Lightfoot**, **Morrison**, **Parsons**) are major users of UKRI facilities (DLS, ISIS, EPSRC Services) as evidenced by the £16M total in-kind funding allocated during the assessment period.

International: access to major international facilities has facilitated the following research: the structure of lead halide perovskites using the *Spallation Neutron Source, Oak Ridge National Lab*/USA (13 days, **Affield**/**Irvine**/**Payne**); **Attfield**'s characterisation of solid-state structures at *ALBA Synchrotron*/Spain (3 days), *FRM-II neutron facility*/Germany (2 days), *Petra III Synchrotron*/Germany (4 days), and *Spring-8/SACLA*/Japan (3 days); **Morris**'s use of the *Advanced Photon Source*, Chicago/USA (4 days) for PDF studies of materials; **Nudelman**'s analysis of inorganic biomaterials at the *Swiss Light Source* (9 days); and **Kirrander**'s use of X-ray free electron lasers to investigate molecular reactivity (Fig. 6) at *SLAC National Accelerator Laboratory*/USA (34 days), *Spring-8/SACLA*/Japan (35 days), and *FERMI Lightsource*/Italy (4 days).

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

Strong and wide-ranging collaborations by EaStCHEM staff, which are enabled by pooled expertise and world-leading research facilities, are demonstrated by an analysis of the 3400 outputs produced since 2014 [*Web of Science* (28/12/2020)]. This shows that 450 outputs have a co-author from another UK chemistry department, 200 have an industrial co-author, and over 1000 are co-authored by a researcher from another discipline. International collaborations have resulted in outputs with co-authors from Europe (820), Asia (470), North America (342), the Middle East (140), Australasia (80), South America (39), and Africa (22).

4a. Research collaborations, networks and partnerships

In addition to many informal collaborations, EaStCHEM's staff play a leading role in interdisciplinary research centres and partnerships at local, national and international level. *Local centres* (Fig. 10) include Proteus (**Bradley**/**Megia-Fernandez**), which has been highlighted by the House of Lords as an exemplary interdisciplinary research hub in which chemists, biologists, optical physicists, designers and clinicians are co-located and work together day-to-day to tackle lung disease. This unique approach has delivered the first optical imaging probes ever used in the human lung (Fig. 5), the first ever to detect bacterial infection *in vivo* in humans, and four chemical reagents now in clinical studies. **T-CBI** research is also incorporated within *The Biomedical Sciences Research Complex* (**BSRC**), forging links with **Biology**, **Physics** and **Medicine**, as well as theme **T-CS** through the EaSICAT Training Centre. The Centre for Magnetic Resonance (**CMR**) links **T-FM** with **T-CBI**. Within **T-SCCD** we lead the *Scottish Centre for Interdisciplinary Surface Spectroscopy* (**SCISS**) that links with **Physics**, while the *Centre for Science at Extreme Conditions* (**CSEC**) links with the Schools of **Physics**, **Engineering**, **GeoSciences** and **Biological Sciences**. Achievements from CSEC includes the demonstration of the first agostic uranium-hydrogen bond formed using high pressure (**Parsons**, *ACIE* **2015**). **T-FM** and **T-EES** researchers collaborate closely with **Physics** via the **Organic Semiconductor Centre** and with **Engineering** on the applications of porous materials and polymer membranes.

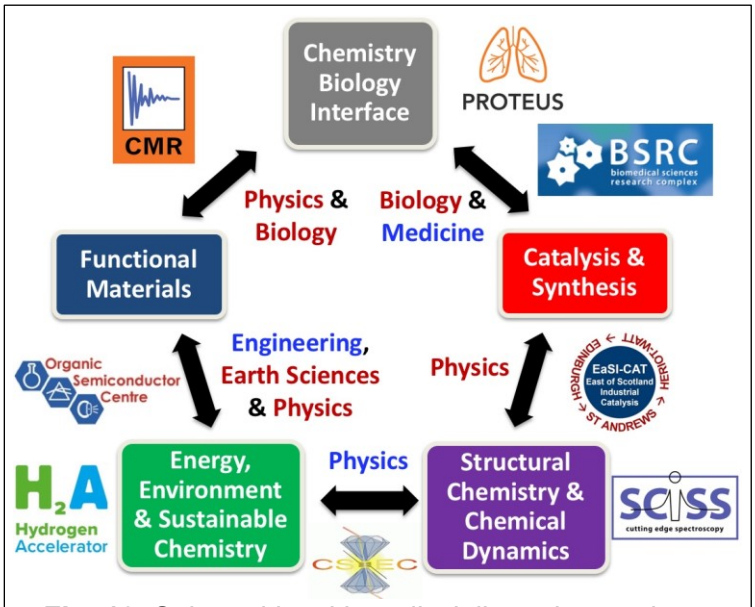

Fig. 10. Selected local interdisciplinary interactions.

As noted in more detail in Section 3a, we are members of a range of research consortia and networks. ***Nationally***, these include large UKRI IRC/Critical Mass/Programme/Platform grants focussed on materials for medical (**Bradley**), magnetic (**Brechin**/**Attfield**), separation membrane (**McKeown**), porous material (**Morris**) and energy (**Irvine**) applications. ***Internationally***, we contribute to research projects across the EU (e.g., *HySeas III*, €13M, **Irvine**; *M4CO2*, €10M, **McKeown**/**Wright**; *CUCAM*, €9M, **Morris**) and at the Eden Campus Energy Demonstrator (European Regional Development Fund/Scottish Enterprise, £1.1M, **Irvine**). We have co-ordinated (*SubiCAT*, *PhotoReact*) and participated (*TADFLife*) in 3 Marie-Curie ITN networks with a combined value of >£7M. Beyond the EU, collaborations are funded by an EPSRC-JSPS Core-to-Core Programme on optoelectronic materials with Kyushu University, Japan (£1M, **Zysman-Colman**) and a US Department of Defense grant with the *Edgewood Chemical Biological Centre* (£1.1M, **McKeown**).

4b. EaStCHEM's contributions to the economy and society not captured by impact case studies

In addition to the seven ICSs, we have generated the following diverse impact.

Industrial/economic impact

- Ongoing collaborations support the development of new processes for *Ingenza*, a spin-out from EaStCHEM research in 2002 (REF2014 ICS), and now a world leader in industrial biotechnology (**Colin Campbell**/**Campopiano**/**Uhrin**).
- Work with *Integrated Graphene*, funded by Innovate UK, resulted in a disruptive manufacturing process of 3D graphene foam electrodes (**Schaub**).
- A fluorescence-based method to reduce transmission of micro-organisms in the poultry *industry* is currently in commercial testing with a major breeder *Aviagen* (**Jones**).
- Optoelectronic materials research has led to a spin-out company *SolOLED* developing solution-processed OLEDs (**Zysman-Colman**).
- Expert support for MS analysis confirmed the absence of carcinogenic residues in pig meat preventing the withdrawal of FDA approval for *Phibro Animal Health Corp*'s leading *Mecadox* antibiotic (**Campopiano**/**Clarke**).
- An enzymatic method for preparing halogenated heterocycles has led to the formation of a spin-out company *XGenix* (**Goss**).
- **Consultancy** has been provided to industry ranging from large international companies (*Afton Chemicals*, *ALMAC, Antabio, Bioven*, *Daiichi-Sankyo*, *ExxonMobil, Mars*, *Merck*, *Pharmaxis Ltd, Servier*, *Syngenta*, *Vertex Pharmaceuticals*) to smaller local ventures (*Cambrex*, *Ingenza*, *Graphene Star*, and *Integrated Graphene*).

Environmental impact

- As a member of DEFRA's *Air Quality Expert Group* and the Department of Health's *Committee on the Medical Effects of Air Pollutants*, **Heal** advises governments on air pollution and its consequences for health. Research, including analysis of ammonia sources and application of ^{14}C dating to airborne particulate matter, has provided valuable evidence of the role of farming emissions and domestic wood burning in the UK. Both are now included in policy action for the first time through the *2019 Clean Air Strategy*. The diffusion-tube guidelines presented in our REF2014 ICS remain the standard for statutory NO_2 measurements across Scotland.
- Research by **Bell** on peatland degradation and restoration at a molecular level informs restoration decisions through advisory roles for the *Scottish Wildlife Trust* (Red Moss of Balerno), *RSPB* (Flow Country, Caithness and Sutherland), and *Global Peatlands Initiative*.
- **Robertson**'s research has informed reports including the *Solar Vision for Scotland* (to Scottish Parliament, 2014), *Solar Commission* report (UK Government, 2019), and the *Review of Innovation and Opportunity in the Scottish Solar Energy Sector* (Scottish Government, 2020).

Health impact

- A fluorescence method that delivers fast and comprehensive antibody analysis forms the basis of *Quotient*'s *MosaiQ* platform for automated testing of blood grouping and infection (**Colin Campbell**). The technology is now in trials and has been rapidly applied to provide a high-performance COVID-19 antibody test, available from April 2020.
- With *Edinburgh Molecular Imaging*, fluorescent labelling of colonic polyps will improve detection and removal of suspect lesions (**Bradley**).
- Alchemical free-energy simulation software for computing binding affinities between proteins and drug-like molecules is commercially available in *Cresset*'s structure-based design tool *Flare* to speed up pre-clinical drug-discovery (**Michel**/**Mey**).
- MS techniques have been developed for the 3D imaging of cell cultures for *AstraZeneca* (**Clarke**), and to characterise a lung cancer vaccine for *Bioven* (**Mackay**; see Section 3b).

Cultural impact

- Advanced chemical analysis of dyestuffs has enabled re-interpretation and enhanced conservation of important textile and quillwork artefacts at museum and gallery partners worldwide (**Hulme**).

Impact on defence and security

- Research on energetic materials in collaboration with *The Falcon Project*, *Weapons Science Technology Centre*, *UK Home Office*, and *US Army*, has influenced UK MOD policy on their

incorporation into munitions (**Pulham**).
- Novel microporous polymeric adsorbents for Chemical Warfare Agents, such as Sarin and Novichok, are being developed in collaboration with the *US Defense Threat Reduction Agency* (**McKeown**).

The COVID-19 crisis has initiated the following research projects: (**1**) fluorescent peptides that selectively label SARS-CoV-2 virions for drug screening and diagnostic applications (**Michel**/**Hulme**); (**2**) using MOFs to provide enhanced filtration by targeting binding of the exterior spike protein of the virus (**Morris**); (**3**) proteins engineered to reduce inflammation in the lungs (**Barlow**); (**4**) oxygen generation by separation from air using either polymer membranes (**McKeown**) or electrochemical generation (**Irvine**); (**5**) repurposing *Sunamp*'s thermal storage technology to provide hot water for mobile hand-washing facilities, and transportation and storage of ultra-cold vaccines for delivery to GPs and care homes (**Pulham**).

4c. Public engagement and outreach

Outreach activities are coordinated by our dedicated Public Engagement/Widening Participation Officers (**Burns**/**Baker**). Top-up funding to PhD scholarships and the CRITICAT/OPTIMA CDT programmes provide a core group of graduate students to develop and deliver activities.

Highlights

- Development of STEM engagement activities to challenge gender stereotypes for pre-school children (Fig. 11). This expertise was shared widely via the *British Interactive Group STEM Communicators Network* Annual Conference (2019).
- At secondary level, the **Chemistry on Tour** and **Chembus** initiatives takes chemistry experiments and demonstrations to >20 schools and communities across Scotland per year focussing on deprived and rural areas that links with RSC local sections.
- Annual **Christmas Lecture series** that gives exciting Chemistry demonstrations to local school students at secondary level.
- An engaging "shooter" computer game (*eXcitune*, **Kirrander**; Fig. 12) communicates complex concepts in theoretical chemistry (*Explorathon* 2017, *Festival of Physics* 2018/2019).
- As part of the **First Chances** programme, National 5/Higher School students have studied the links between the structure of molecules and their fragrance, as well as renewable energy and fuel cell technology (**Aitken**/**Baker**).
- Use of virtual reality software to introduce young people to biomacromolecular structures (**Michel**, Edinburgh Science Festival, 2019).
- Proteus (**Bradley**/**Megia-Fernandez**) with public engagement strategist, Helen Szoor-McElhinney, has produced the *Circuits!* teaching tools to inspire the next generation of biomedical engineers based on a working model of their optical imaging technology. This is now incorporated into the Scottish high school curriculum, and has a permanent pod in the *Glasgow Science Centre*.

Fig. 11. STEM outreach for pre-school children.

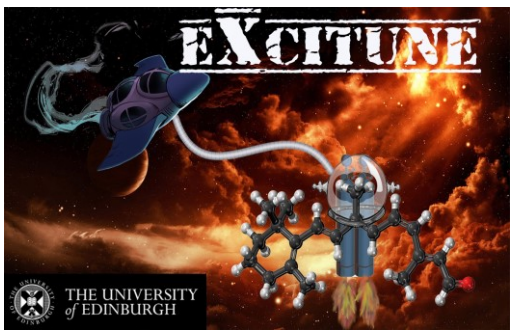

Fig. 12. The computer game *eXcitune*.

Examples of EaStCHEM promoting chemistry via the mass media include discussing the recently discovered **UStA** periodic table on *Antiques Road Trip* (**O'Hagan**), plastic sustainability and urban mining on BBC Radio Scotland's *Brainwaves* (**Garden**, **Love**, **McKeown**), solar water treatment in rural India on *Radio Scotland* (**Robertson**), and the photoprotection of antibiotics with pollen with Radio 4/*The Times* (**Goss**).

4d. Contributions to the sustainability of the discipline

EaStCHEM researchers contribute significantly and diversely to the sustainability of chemistry, as illustrated by the following examples.

Promotion of women in chemistry and STEM: "*A Chemical Imbalance*", (*www.chemicalimbalance.ed.ac.uk),* which features **Arnold**, **Eleanor Campbell**, **Hulme**, **Jones**, and **Morrison**, is a call to action for simple changes to achieve equality of opportunity in science. **Arnold** also launched a new network for senior women in STEM in Scotland, *SciSisters*. **Ashbrook** has authored the "*Academic Women Now*" and "*Academic Women Here*" booklets, describing the experiences of mid-career academic women in Scotland.

Chemical education: **Seery**'s pedagogical research provides insights on how chemistry students interact with the curriculum outside of formal lectures to enhance self-learning, which informs his very popular *YouTube* video channel (passed 1M views on 06/10/20).

Major contribution to UK chemistry committees: President of the RSC Faraday Division (**Eleanor Campbell**, 2015-18); President of the RSC Perkin Division (**Hulme**, 2017-20); Chair/Treasurer of the RSC Theoretical Chemistry Group (**Morrison**/**van Mourik**); Chair of the RSC Heterocycle and Synthesis Group (**Smith**, 2020-current); Chair of the RSC Inclusion and Diversity Committee (**Arnold);** Chair of Heads of Chemistry UK (**Eleanor Campbell**, 2013-15; **Pulham**, 2019-21).

4e. Indicators of wider influence

In addition to scientific advisory panels that drive policy change (Section 4b), EaStCHEM's researchers have contributed to the following national/international panels/committees.

EPSRC Physical Sciences Prioritisation (**Bradley**, **Lusby**, **O'Hagan**, **van Mourik**); EPSRC Programme Grants (**Bradley**, **Hulme**, **O'Hagan**, Chair); EPSRC New Horizons (**Bradley**); ERC Starter/Consolidator Fellowships PE4/5 (**Arnold**, **Ashbrook**, **Bradley**, **Zysman-Colman**); ERC Synergy Grants Evaluation (**Eleanor Campbell**); Leverhulme Trust Prize (**Morris**, **Eleanor Campbell**); Blavatnik Awards for Young Scientists, UK Jury (**Eleanor Campbell**); STFC Advisory Panel for Public Engagement (**Pulham**, Chair); RS APEX/FLAIR Committees (**Morris**); RS Wolfson Fellowship (**Lloyd-Jones**, **Eleanor Campbell**); RS URF (**Eleanor Campbell**, Chair; **Lloyd-Jones**, **Slawin**); RS Newton International Fellowships (**Ashbrook**); Swedish Research Council Grant Review (**Eleanor Campbell**; **Hulme**); STFC scientific panel that prepared the science case for the UK X-ray free electron source laser (**Kirrander**).

4f. Recognition by the research base to EaStCHEM researchers

Fellowships: the ***RS*** elected **Arnold**, **Attfield**, **Morris** and **Naismith** as Fellows, to join existing FRSs **Eleanor Campbell** and **Lloyd-Jones** and provided **Ashbrook**, **Lloyd-Jones**, and **Smith** with Wolfson Merit Awards. The ***RSE*** elected **Ashbrook**, **Goss**, **Lloyd-Jones**, **McKeown** and **Smith** as Fellows, and appointed **Ashbrook**, **Johansson** and **Thomas** as members of the Young Academy of Scotland. **Morris** is RSE Vice-president (physical sciences and engineering); **Eleanor Campbell**, **Morris** and **Irvine** were elected Members of *Academia Europaea* and **Attfield** Fellow of the *Indian National Science Academy*.

RSC Awards and Prizes: Joseph Black Award (**Bell**, 2017); Chemistry of the Transition Metals Award (**Brechin**, 2014); Bob Hay Lectureship (**Cockcroft**, 2017); Corday-Morgan (**Ashbrook**, 2015); Tilden Prize (**Lloyd-Jones**, 2014; **Bradley**, 2015; **McKeown**, 2017; **Brechin**, 2018; **Morris**, 2019); Sustainable Energy Award (**Irvine**, 2015); Peter Day Award (**Morris**, 2015); Organic Stereochemistry Award (**O'Hagan**, 2015); Interdisciplinary Prize (**Bradley**, 2019); Merck Award (**Smith**, 2014); Hickinbottom Award (**Thomas**, 2016; **Lawrence**, 2017; **Watson**, 2019); Charles Rees Award (**Smith**, 2018); Pedlar Award (**Lloyd-Jones**, 2018), Emerging Technology Award (**Morris**, 2016); Wilkinson Prize (**Arnold**, 2018); and Capps Green Zomaya Memorial Award (**Michel**, 2020); RSC Industry and Technology Award (**Mowat**, 2016).

Other significant national prizes: RSE Sir Thomas Makdougall Brisbane medal (**Cazin**, 2014); Philip Leverhulme Prize (**Cockroft**, 2016); Ubbelohde Prize, British Carbon Group, (**Eleanor Campbell**, 2016); Suffrage Science Award (**Arnold**, 2015; **Ashbrook**, 2017); RSE Lord Kelvin Medal (**Arnold**, 2017; **Irvine**, 2018); Durward Cruickshank Young Crystallographers' Prize

(**Hobday**, 2018); CCDC Chemical Crystallography Prize for Younger Scientists (**Hobday**, 2018); Macro Group Young Investigators Award (**Garden**, 2019).

International awards: Federation of Analytical and Spectroscopic Societies Innovation Award (**Colin Campbell**, 2015); The Baron Axel Cronstedt Award (**Morris**, 2017); EuCHEM Young Investigator (**Watson**, 2018); Prix Moissan of the Maison de La Chimie (**O'Hagan**, 2018); L'Oréal -UNESCO For Women in Science Fellowship (**Garden**, 2019); Mercator Fellowship of the Deutsche Forschungsgemeinschaft (**Morris**, 2018); Anders Gustaf Ekeberg Tantalum Prize (**Love**, 2020).