High End Computing Consortia Annual Report Guidance 2018-2019

Introduction

The overall vision for ARCHER is for the UK to be a recognised leader on the international scene for computational science and engineering. In order to achieve this, UK researchers must be able to carry out internationally competitive research across the remit of EPSRC and NERC. The Full Business Case for ARCHER gives the key benefits from the establishment of the next generation national high performance computing service. In summary these are:

- World-class and world-leading scientific output
- Greater scientific productivity
- Training support for graduates and post doctorates
- Increase in the UK's computational science and engineering skill base
- Increased impact and collaboration with industry (updated to recognise 'Impact' of HPC across the wider economic, societal and environmental metrics)
- A strengthening of the UK's international position for producing world-class science.

EPSRC must therefore work closely with ARCHER users in their community to fully understand the benefits and impact of the ARCHER service. As ~65% of EPSRC's ARCHER resource is currently allocated *via* eight EPSRC supported High End Computing (HEC) Consortia it is essential that the Consortia to provide key information on the benefits of the service. These Consortia are:

- Material Chemistry Consortium (MCC)
- UK Turbulence Consortium (UKTC)
- UK Car-Parrinello Consortium, (UKCP)
- Biomolecular Simulation Consortium (HEC BioSim)
- Plasma Physics Consortium, (PPC)
- UK Mesoscale Engineering Consortium (UKCOMES)
- UK Turbulent Reacting Flows Consortium (UKCTRF)
- UK Atomic, Molecular and Optical Physics R-matrix Consortium (UKAMOR)

Outputs

This Annual Reporting template for has been designed around the existing SLA reporting template and the headings outlined in the ARCHER benefits realisation plan. The Annual Reports will be shared with both the SLA Steering Committee and the ARCHER Strategic Management Board for information and comment. The annual reports will also provide content for the Consortia pages on the ARCHER website.

This year's Annual Reports will **NOT** be formally assessed and will **NOT** influence ARCHER allocations. The focus of these Annual Reports will be to capture evidence of the impact of the Consortia and ARCHER.

Timeline 2019:

- **Deadline for Annual Reports:** Friday 15th November 2019
- **SLA Steering Committee:** Wednesday 15th January – Q1 2020
- **ARCHER Strategic Management Board Meeting:** TBC but in Q1 2020

Annual Report for EPSRC High End Computing Consortia

Reporting Period: November 2018 – October 2019

HEC Consortium: Materials Chemistry HEC Consortium (MCC)

Consortium Chair: Prof. Scott M. Woodley

Allocation and Usage profiles during the reporting period
EPSRC to complete when template has been submitted.
Summary (max. 2 pages):

Background

The Materials Chemistry Consortium (MCC) covers the modelling and prediction of the structures, properties and reactivities of materials. The emphasis is on modelling at the atomic and molecular level but with links to models at larger length and time scales. The MCC has an active programme of code development and optimisation, supported by COSEC and EPSRC software initiatives. A wide range of techniques is used: both force-field methods employing static and dynamical simulation methodologies and electronic structure methods with a strong emphasis on Density Functional Theory (DFT) techniques using both periodic boundary condition and embedded cluster implementations. The current scientific programme embraces five themes on applications and three on fundamental aspects of materials, bringing together the best minds of the UK academic community who represent over 25 universities. Close collaboration and scientific interactions between our themes will promote rapid progress and advancement of novel solutions benefiting both applied and fundamental developments.

Workshops and New Opportunities

Since our last report, the MCC has investigated the opportunities that Quantum Computing may offer our and other similar communities. Sponsored by CCP5, CCP9, CCPBiosim, Q-LABS and of course ourselves (MCC), we organised a one-day meeting, entitled "Scientific Applications of Quantum Computing" at a neutral London venue (LSE Bankside) on the 14th May. The event attracted over 85 registered participants from science, quantum computing, government and commercial sectors. The morning consisted of a series of talks covering current state of play (algorithms, soft- and hardware capabilities in both science and quantum computing) and the scientific challenges we want to address. The afternoon was devoted to discussions around three key questions: (1) What are the potential scientific opportunities in the different fields represented at the meeting? (2) How do we promote collaborations between different scientific and quantum computing communities? (3) What mechanisms are needed to make progress? One of the main conclusions of this event was the importance of creating a new CCP for this area; hence, an application for the creation of CCPQC has been submitted to EPSRC's current CCP call.

For 2020 we plan to hold our third 3-day MCC conference, this time in Daresbury, where members of our consortium will showcase, to an international panel of experts, recent scientific research made possible from access to Tier-1 and 2 HEC resources and complimentary software development. We also plan to run a number of smaller workshops, including one on *heterogeneous catalysis* and another on *materials based on Perovskites* as well as a user workshop for the new release of CHEMSHELL.

We have obtained RS Hooke funding to run a discussion meeting on *Supercomputer modelling of advanced materials* at the Royal Society 14-15 September 2020, which will be followed by a satellite meeting, 16-17 September 2010, that will focus on the software solutions to the challenges discussed during the main meeting. More details will be posted by the Royal Society.

Issues and Problems

No new issues or problems to report.

Membership

The consortium is a large but coherent grouping with over 600 registered users on ARCHER (around 120 new users since our last report) and over 125 registered users on THOMAS from 80 research teams based in 30 institutions.

New member joining during the 18/19 reporting period: Constantinos D Zeinalipour-Yazdi (Greenwich).

Other members joining during ARCHER service: Arunabhiram Chutia (Lincoln), Clotilde Cucinotta (Imperial College London), Livia Bartok-Partay (moved from Reading to Warwick), Reinhard Maurer (Warwick), Jonathan Skelton (Manchester), J Axel Zeitler (Cambridge), Sanliang Ling (Nottingham), Rachel Crespo-Otero (Queen Mary, London), Francesca Baletto (Kings College London), Matthew Addicoat (Nottingham Trent), Alberto Roldan (Cardiff), Paul Bristowe (Cambridge), Ian Bush (Oxford), Stephen Elliot (Cambridge), Andrea Floris (Lincoln), Steven Hepplestone (Exeter), Denis Kramer (Southampton), Andrew Logsdail (Cardiff), Natalia Martsinovich (Sheffield), Marco Molinari (Huddersfield), Paul Mulheran (Strathclyde), Samuel Murphy (Lancaster), Michail Stamatakis (UCL), Jin-Chong Tan (Oxford), Stanko Tomic (Salford), Nikolas Kaltsoyannis (Manchester), Alberto Striolo (UCL), Matthew Watkins (Lincoln), Marc-Oliver Coppens (UCL), Johannes Lischner (Imperial), Benjamin Morgan (Bath), Ian Shuttleworth (Nottingham Trent), David Scanlon

(UCL), Marco Sacchi (Surrey), Chris Lorenz (KCL), Sally Price (UCL), Graeme Watson (Dublin), Devis Di Tommaso (QMUL), Jamieson Christie (Loughborough), Kim Jelfs (Imperial), and Stefano Leoni (Cardiff).
Members since before the ARCHER service:
Furio Cora (UCL), Paul Elliot (Huddersfield), Colin Freeman (Sheffield), John Hanna (Warwick), Sanghamitra Mukhopadhyay (STFC), Matthew Foulkes (Imperial), Mark Read (Birmingham), Pooja Panchmatia (Loughborough), Graeme Day (Southampton), Keith McKenna (York), Mats Persson (Liverpool), Maria Alfredsson (Kent), Aron Walsh (Imperial), David Cooke (Huddersfield), Jochen Blumberger (UCL), George Darling (Liverpool), Clare Grey (Cambridge), Kostya Trachenko (QMUL), Martijn Zwijnenburg (UCL), Barbara Montanari (STFC), Arash Mostofi (Imperial), Ricardo Grau-Crespo (Reading), Antonio Tilocca (UCL), Roy Johnston (Birmingham), Dorothy Duffy (UCL), Lev Kantorovitch (KCL), Angelos Michaelides (UCL), Martin Dove (QMUL), Stephen Parker (Bath), Nora de Leeuw (Cardiff), Ben Slater (UCL), John Harding (Sheffield), Alex Shluger (UCL), Saiful Islam (Bath), David Willock (Cardiff), Nicolas Harrison (Imperial), Scott Woodley (UCL), and Richard Catlow (UCL, Cardiff).
Institutions include: Bath, Birmingham, Cambridge, Cardiff, Dublin, Exeter, Greenwich, Huddersfield, Imperial College, Kent, Kings College London, Lancaster, Lincoln, Liverpool, Manchester, Nottingham, Nottingham Trent, Oxford, Queen Mary University London, Reading, Salford, Sheffield, Southampton, STFC, Strathclyde, Surrey, University College London, Loughborough, Warwick, and York.
Change to executive committee during the 18/19 reporting period: Dorothy Duffy has been replaced by Aron Walsh (joins Saiful Islam to oversee the Application Theme of Energy Generation, Storage and Transport) and Roy Johnston (Nano Theme) who tragedly passed away during the Summer.

World class and world leading scientific output: *ARCHER should enable high quality and world-leading science to be delivered. This should generate high impact outputs and outcomes that increase the UK's position in world science.*

Publications

All members of the MCC are requested to acknowledge the MCC and EPSRC as well as the grant number EP/L000202 and/or EP/R029431 for all publications that benefited from membership of the MCC and resources allocated under e05 on ARCHER. Simillarly for all publications that benfited from membership of the MCC and resources allocated on THOMAS, including the grant number EP/P020194. Furthermore, once published, details of the articles are to be uploaded into our online Google Spreadsheet. All new entries are then entered into ResearchFish by the end of the ResearchFish reporting period. To date we have 122 and 83 publications for 2018 and 2019, respectively, listed in our database, fourteen of which have co-authors from industry and one hundred and ten with co-authors based outside the UK.

Scientific Output

The broad but coherent work of the consortium is divided into themes, each led by two members of our executive committee. All have shown novel, world leading scientific achievements during the last year as summarised below.

Reactivity and Catalysis [Theme Leaders: David Willock (Cardiff) & Richard Catlow (UCL)]
The reactivity theme covers a wide range of chemical transformations involving solids and their surfaces. There is an emphasis on the area of heterogeneous catalysis as one of the main UK drivers for research into the adsorption and reaction of molecules over surfaces. In this area the aim is to make links between the material properties and the ability of the material to catalyse target reactions in order to reduce energy consumption and to improve productivity and reduce environmental impact. A very general way to classify surface features is through geometric descriptors and researchers within the consortium have shown how such descriptors can be used to understand the activity of metal particles for the electrocatalytic oxygen reduction reaction following the structure of supported metal particles as function of time and temperature[1,2]. Direct studies of catalytic processes over surface has also lead to the discovery of a role for PdN_x species in the oxidative removal of ammonia from pollution streams[3] and detailed insights into the mechanistic steps involved in the conversion of methanol to gasoline over zeolite materials[4].

Materials for Energy Generation, Transport & Storage [Theme Leaders: Saiful Islam (Bath) & Dorothy Duffy (UCL)]

There has been considerable progress in advanced computational studies of functional materials for energy storage and energy conversion using the ARCHER facilities. Materials performance lies at the heart of the development and optimisation of energy devices. Important challenges include increasing the energy density and charge rate of lithium and sodium batteries – vital factors for battery use in next-generation portable electronics, electric vehicles and grid storage. The breadth of the computational work is evident from the following selection of scientific highlights:

- Developing new solid electrolyte materials is crucial for safer all-solid-state batteries. Using two model electrolyte systems, Na_3PS_4 and Na_3PO_4, a novel microscale simulation approach was applied to analyse ionic transport in polycrystalline materials with various grain volumes. For Na_3PO_4, high grain boundary resistance is found, whereas, for Na_3PS_4, the overall influence of grain boundaries (GBs) is significantly reduced compared to the oxide. Detailed analysis reveals significant differences in the local structures and Na-ion conduction mechanism and helps to explain the fundamentally different influences of GBs on ion transport in phosphate and thiophosphate solid electrolytes [5];
- A number of absorber materials are being actively developed as the basis for next generation solar cells. These include a range of lead halide perovskites as well as binary materials such as CdTe. Unlike the incumbent silicon, all of the materials are polycrystalline and therefore the properties of extended defects such as grain, twin and antisite boundaries has become an important topic. Density functional theory is used to model the structure, stability and electronic properties of stable extended defects in CdTe and a number of lead halide perovskites. These results provide insight into their electronic properties, which will be used to guide the optimisation of better performing absorbers for solar cell applications [6];
- Thermoelectric (TE) power allows waste heat to be recovered as electricity and is an important technology for improving the efficiency of energy-intensive processes. Alloying is a common strategy for reducing thermal conductivity, but the microscopic mechanisms are not well understood. New work on the Sn(S,Se) system, one of the current flagship TE materials, is a pilot study aiming to develop the theoretical methodology required to address this. Oxide TEs are highly desirable for their low cost and abundance, and work on the Ti_nO_{2n-1} system has indicated these materials to be promising candidates for efficient, low-cost TEs. Our modelling work has informed ongoing experimental work and provides insight that may allow other potential oxide TEs to be identified in the future [7].

Environmental and Smart Materials [Theme Leaders: John Harding (Sheffield) & Nicholas Harrison (IC)]

In the past year this theme has made progress in four key areas.

- Simulations of radiation damage has been performed for in candidate materials for nuclear waste encapsulation. The nature of high-energy radiation damage in glassy materials has been quantified for the first time. This was achieved by running high-energy recoils in amorphous structures of silica and zirconolites. This is part of a partnership between Queen Mary University of London and the United Nations International Atomic Energy Agency (IAEA);
- Mineral carbonation of carbon dioxide (CO_2) represents a very promising and long-term solution for the use of captured and stored anthropogenic CO_2. One of the potential product of mineral carbonation is magnesite ($MgCO_3$). However, its precipitation under ambient conditions is slow. Simulations on the dehydration of Mg^{2+} ions (the rate-determining step in precipitation of $MgCO_3$) have been performed [8] as part of a new project “Fundamental studies of mineral carbonation with application to CO_2 sequestration”;
- Rare earths are on the European Union list of critical minerals. The solid and liquid speciation and the local structure ofyttrium have been studied in high-sulphate aqueous solutions,basaluminite standards, and samples from remediationcolumns using synchrotron-based techniques and molecular modelling [9]. The results are an essential starting point for work on rare earth recovery from waste generated in acid mine drainage remediation systems;
- The photo-switching capabilities of hemithioindigo and derivative molecules on an Ag(111) substrate have been studied both computationally and experimentally. These have high potential for

controlling molecular processes in materials and biomolecular sciences. The simulations show that the molecules are likely to adsorb extremely close to one another in varying orientations. Understanding this is the starting point to elucidating the electronic structure of the interface and hence developing a blueprint for organic semiconductor-based single-molecule optoelectronic devices.

Soft Matter and Biomaterials [Theme Leaders: Chris Lorenz (KCL) & Jamie Christie (Loughbough)]

In this theme, there is a significant amount of research being conducted investigating the materials-biology interface.

- Over the past year, in collaboration with a pump-probe experimental group at UEA, significant contributions in understanding the electron transfer mechanism within the tetra-heme protein STC junction between gold leads have been made [10]. In another multi-disciplinary study, adding one methane (-CH2-) group to the functional group of the molecules in a self-assembled monolayer, was shown to modify the interfacial hydration layer enough to change completely the structure of an adsorbed layer of fibronectin proteins [11], providing a fundamental understanding of the tissue engineering platform used to regenerate bone for severely injured animals [12].
- Hybrid materials which incorporate both nano and biological material are also the focus of a significant amount of work within this theme. For example, this year a new metal-organic framework composed of zinc ions and tripeptide molecules was synthesised and shown to adopt nine crystal structures in a variety of solvents. By controlling the solvents to which the material was exposed, the researchers were able to trigger uptake of particular guest molecules and simulations could rationalise the behaviour in terms of the host potential energy surface and its perturbations caused by the guest-host interactions [13].
- In the area of soft matter, the self-assembly of various types of drug delivery formulations have been the focus of a significant work. Large-scale molecular dynamics simulations and neutron scattering experiments combine to provide a detailed description of the molecular structure of solid lipid nanoparticles, how the molecules transition their structure within the particles, and the mechanisms by which they encapsulate drugs [14]. Additionally, researchers have used an in house non-adiabatic dynamics code to investigate the direct propagation of the electron and nuclei and to deliver an “ab initio” view into the charge transport mechanism, which proved to be a useful tool to measure charge mobility in these systems [15, 16].
- This year, a lot of work has been done investigating the mechanism of action of antimicrobial peptides, which are of significant interest as a potential method to counter antimicrobial resistance, and how this mechanism changes with very minor changes in the sequence of the peptides [17,18].

Materials Discovery [Theme Leaders: Graham Day (Southampton) & Kimberly Jelfs (Imperial College)]

The Materials Discovery theme aims to use simulations to accelerate the discovery of new materials, including porous materials and organic electronics. This includes a strong relationship with experimental collaborators, who are testing predictions in the laboratory. Specific examples include:

- *Benchmarking stabilities of experimental organic co-crystals.* Solid-state density functional theory calculations were used to quantify crystal stabilisation and rationalise observed packing tendencies in a statistically-representative benchmark.[19]
- *Crystal structure prediction of porous materials for molecular separations.* ARCHER was used for crystal structure prediction calculations to understand the polymorphic landscape of a pillarene, assisting in the rationalisation of the industrially relevant xylene isomer separation.[20]
- *Charge-carrier mobilities in organic molecular crystals*. Charge transport in an organic semiconductor model was simulated to assist in the development of a code for non-adiabatic molecular dynamics.[21]

Fundamentals in Bulk Properties [Theme Leaders: Alex Shluger (UCL) & Keith McKenna (York)]

Highlights within this theme include:

- Boron arsenide, BAs, has an unusually high thermal conductivity, comparable to diamond and far higher than the typical materials used in high power microelectronics, where efficient heat transfer is crucial to avoid device malfunction. Calculations employing high level multiparticle methods and excited states have predicted the electronic properties of BAs and provided a set of material

properties which will help guide future experimental work [1];

- Understanding mechanisms of dielectric breakdown is important technologically important electronic devices such as transistors and resistive switching memories. New atomistic mechanisms of degradation of crystalline and amorphous SiO_2 and HfO_2 films in electronic devices under application of electric field and electron injection conditions were developed in [2-4].
- A new methodology established previously in SiO_2 was used to predictively model the structure, defect properties and electron and hole trapping in amorphous SiO_2, ZnO, Sm_2O_3, Al_2O_3 [5-11] finding good agreement with experimental spectroscopic data.
- Hexagonal boron nitride (hBN) is a wide gap 2D layered material with good insulating properties. Calculations using hybrid density functional theory predicted the structure and properties of a wide range of intrinsic point defects in the bulk of hBN. These results provide further insight into the properties of defects which can be responsible for degradation of hBN based devices [12].
- The structural and electronic properties of Y_2O_3 doped HfO_2 were statistically modelled using hybrid density functional approach. The cubic phase of HfO_2 was predicted to be stabilised for doping concentrations near to 12.5 at. %, and the gap was free from charge trapping defect states This makes Y doped HfO_2 a suitable high-dielectric constant material for complementary metal-oxide semiconductor applications. [13]

Fundamentals in Surfaces and Interfaces [Theme Leaders: Ben Slater (UCL) & Matthew Wattkins (Lincoln)]
Scientific outputs within this theme include:

- Chiral molecular walkers can diffuse on an anisotropic achiral surface towards a preferential direction under the influence of an external oscillating stimuli (external field or temperature gradient) [35]. The results obtained in this work show a natural mechanism in which, under certain conditions, one enantiomer moves towards one direction, while the other - in the opposite one, separating them. This is very interesting, because all living beings are homochiral (composed by only one of the two possible enantiomers). We hope that this result may shed some light in answering fundamental questions of the origin of life, as well as of the emergence of homochirality.
- UiO-66 network was studied [36] using groundbreaking HRTEM imaging and state of the art DFT to establish the atomic structure of defect centres in this water and thermally stable Metal Oorganic Framework. The motivation behind this work was to establish, with atomic precision, what the defect structures look like, since the presence of defects in this material is known to facilitate catalysis, such as epoxidation reactions. Not only were these active centres resolved for the first time, the distinct role of these defects in catalysis was unpicked.
- Many papers continue to demonstrate the benefits of strong links between theory and experiment e.g. [37-40].

Fundamentals in Low Dimensional Materials [Theme Leaders: Roy Johnston (Birmingham) & Scott Woodley (UCL)]
This is a new distinct theme in our consortium that brings together research in matter organised at nanoscale of different dimensionality. Discovering the commonality in physical and chemical effects of vastly divergent materials and applications as well as the whole plethora of novel structures and has heightened the interest in materials community, led to the development of new approaches. The dedicated effort by MCC members in the last year yielded a number of insightful and exciting results both of fundamental and applied interest, some of which are highlighted below.

- Self-assembly of copper heterostructures on black phosphorus multilayers: The electronic and atomic structure of atomically thin chiral copper heterostructures templated by black phosphorus was unravelled by a collaboration between experimental and theoretical groups. The findings of this new hybrid material with unique dimensionality, chirality, and metallic nature and its triggered self-assembly open new and exciting opportunities for next generation, self-assembling devices [41];
- Modelling of 2D and 3D tin-based perovskites and their defect-induced optoelectronic properties: Two-dimensional (2D) halide perovskites have recently emerged as stable and versatile family of light harvesting materials for solar cells. They can play various roles within a solar cell device, either as the primary light absorber, as a capping layer, passivating layer, or within a mixed 2D/3D perovskite solar cell absorber. DFT simulations allowed to investigate the effect of layer thickness and defect engineering on

the band gap of these 2D systems. The band structure analysis showed small electron and hole carriers effective masses, suggesting high carrier mobilities. The symmetry breaking due to the distorted structure associated with the orientation of the cations in the perovskite layers is found to be the driving force for the induced Rashba spin-splitting bands in the systems with more than one-layer thickness. 2D perovskites are found to function as hole transport materials when interfacing the 3D analogues.

- Continuing development of new global optimisation techniques for sub-nanometre metal clusters in gas phase and supported on surfaces allowed us to generate structures for further investigation by DFT and Time Dependent-DFT calculations – enabling rationalisation of various experimental electrostatic and magnetic deflection measurements; IR and UV photodepletion spectra (Darmstadt collaboration). This has so far resulted in 18 joint publications with the Schäfer group, focusing on the Darmstadt photodissociation experiments in several studies with the help of ARCHER allocations through MCC.
- A new class of carbon nanostructures at a lower sub-nano end of the size scale with a surprising stability, as compared to the well-known carbon fullerenes, are reported. The octahedral carbon clusters contain tetragonal rings, which, in spite of a common belief, prove to be an energy efficient means of plying graphene sheets to make threedimensional spheroid shapes, similar to fullerenes. The two families of structures are shown to be competitive at small sizes (20 atoms) at room temperature, and for higher temperatures, at both small and large sizes (>200 atoms). Our calculations demonstrate that both vibrational and electronic spectra of these cluster families are similar, which thus might cloud their experimental identification. We propose octahedral clusters and other structures containing tetragonal rings as viable structural elements and building units in inorganic chemistry and materials science of carbon along with fullerenes [42].

References

[1] K. Rossi et al. *PCCP*, 2019, **21**, 4888; [2] K. Rossi et al. *ChemPhysChem*, 2019, **20**, 1-9; [3] E. K. Dann et al. *Nature Catalysis*, 2019, **2**, 157-163; [4] S. K. Matam et al. *Chem. Commun.*, 2018, **54**, 12875–12878; [5] *10.1021/acs.chemmater.9b01794*; [6] K. P. McKenna, *ACS Energy Lett.*, 2018, **3**, 11; [7] D. S. D. Gunn et al. *Chem. Mater.* 2019, **31** (10) 3672-3685; [8] X. Zhang et al. *Eur. J. Min*. 2019, **31**, 27; [9] A. Lozano et al. *Env. Sci. & Tech.*, 2019, **53**, 11153; [10] J. H. van Wonderen et al. *J. Am. Chem. Soc.*, 2019, **141** (38), 15190-15200; [11] M. K. Bieniek et al. *Adv. Theory Simul.*, 2019, doi:10.1002/adts.201900169; [12] https://www.bbc.co.uk/news/uk-scotland-glasgow-west-40366645; [13] A. P. Katsoulidis et al. *Nature*, 2019, 213-217; [14] D. L. Pink et al. *Small*, 2019, **15**, 1903156; [15] S. Giannini et al. *J. Phys. Chem. Lett.*, 2018, **9** (11), 3116-3123; [16] S. Giannini et al. *Nat. Comm*., 2019, **10**, 3843; [17] G. Manzo et al. *Sci. Rep.*, 2019, **9** 10934; [18] G. Manzo et al. *Sci. Rep.*, 2019, **9**, 1385; [19] E. N. Pinter et al., *CrystEngComm*, 2018, **20**, 4213-4220; [20] K. Jie et al., *J. Am. Chem. Soc.,* 2018, **140**, 22, 6921-6930; [21] S. Giannini et al., *J. Phys. Chem. Lett.* 2018, **9**, 11, 3116-3123 [22] J. Buckeridge et al., *Phys. Rev. Materials*, 2019, **3**, 051601R; [23] D. Z. Gao, *Front. Phys.* 2019, **7**, 43; [24] 10.1109/IIRW.2018.8727085; [25] J. Strand et al., *J. Chem. Phys.* 2019, **150**, 044702; [26] E. Olsson et al., *Comp. Materials Sci.*, 2019, **169**, 109119; [27] J. Cotton et al., *ACS Appl. Mater. Interfaces*, 2019, **11** (39) 36232-36243; [28] K. Patel et al., *Microelectronics Reliability*, 2019, **98**, 144-152; [29] O. Dicks et al., *Nanotecnology*, 2019, **30**, 20; [30] D. Mora-Fonz et al., *Phys. Rev. B*, 2019, **99**, 014202; [31] D. Z. Goa et al., *Front. Phys.* 29 March 2019; [32] 10.1109/IPFA.2018.8452536; [33] 10.1088/1361-648X/ab4e5d; [34] A. C. M. Padilha et al., *J. Appl. Phys.*, 2019, **126**, 08105; [35] D. Abbasi-Pérez et al. *Chem. Sci.*, 2019, **10**, 5864-5874; [36] L. Liu et al. *Nat. Chem*. 2019, **11**, 622–628; [37] C. Lin et al., *J. Am. Chem. Soc*. 2018, **140** (46), 15804-15811; [38] M.Bhadra et al., *J. Am. Chem. Soc*. 2019, **141** (15) 6152-6156; [39] P. Wang et al., *Angew. Chem. Int*. 2019, **131**, 16069; [40] A. Khayum et al. *Chem. Sci*. 2019, **10**, 8889; [41] 10.1002/adfm.201903120; [42] T. Lazauskas et al., *Nanoscale Adv.*, 2019, **1**, 89.

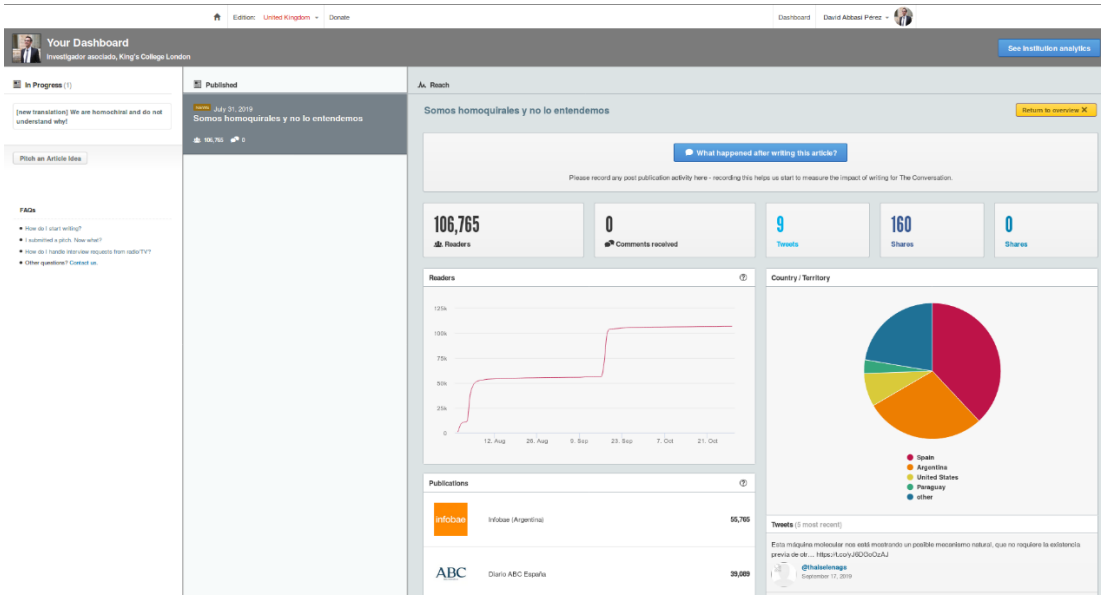
Press Announcements/Other Communications of Significance to an International Community.

The work of the consortium has received attention from the media with the following as examples:

- Publication DOI:10.1039/C9SC01135H was retweeted by Fraser Stoddart, a Nobel laureate for his work on molecular machines. Furthermore, an outreach article was published in the Spanish edition of The Conversation (http://theconversation.com/somos-homoquirales-y-no-lo-entendemos-119101), with the title: “Somos homoquirales y no lo entendemos”, where the results of the research are succinctly explained in a language as plain as possible and engaging. Many media republished the article, including the national Spanish newspaper ABC (https://www.abc.es/

ciencia/abci-eres-homoquiral-y-posiblemente-no-sepas-201908040136_noticia.html), one of the biggest in Spain, reaching more than 100.000 readers all over the world. An English version of the article has been submitted and we hope it will also be published. The current statistics for The Conversation readers who read the article is just under 107K across most of the Spanish-speaking countries as shown in the figure below.

- News highlighted about "Scientists design new responsive porous material inspired by proteins", see: https://www.liverpool.ac.uk/chemistry/news/articles/scientists-design-new-responsive-porous-material-inspired-by-proteins/
- Radio 4 podcast, Professor Saiful Islam talks to Jim Al-Khalili about his life and work studying the materials that make renewable energy possible, see: https://www.bbc.co.uk/programmes/m0009rhg
- Expecting a press release by Univeristy of Warwick this month about a Nature Communications article that will be published under DOI: 10.1038/s41467-019-12875-2.
- Work on defects in metal-organic frameworks using a combination of computational and experimental techniques, a collaboration with colleagues from King Abdullah University of Science and Technology in Saudi Arabia, was published in Nature Chemistry (https://www.nature.com/articles/s41557-019-0263-4) and highlighted by phys.org website, see: "Imperfection is OK for better MOFs" https://phys.org/news/2019-05-imperfection-mofs.html
- The work in publication 10.1039/c8na00013a was highlighted by Alex Metherell in Chemistry World (28 January 2019) in an article entitled "Calculations suggest octahedral carbon clusters more stable than expected".
- Results of an investigation were published as the cover of the flagship journal of the Royal Society of Chemistry, Chemical Science, with an impact factor of 9.556. The paper has an Altmetric score of 51, which is in the top 5% of all research outputs scored by Altmetric. The publication DOI:10.1039/C9SC01135H was retweeted by Fraser Stoddart, a Nobel laureate for his work on molecular machines. Furthermore, an outreach article was published in the Spanish edition of The Conversation (http://theconversation.com/somos-homoquirales-y-no-lo-entendemos-119101), with the title: "Somos homoquirales y no lo entendemos", where the results of the research are succinctly explained in a language as plain as possible and engaging. Many media republished the article, including the national Spanish newspaper ABC (https://www.abc.es/ ciencia/abci-eres-homoquiral-y-posiblemente-no-sepas-201908040136_noticia.html), one of the biggest in Spain, reaching more than 100,000 readers all over the world. An English version of the article has been submitted and we hope it will also be published. The current statistics for The Conversation readers who read the article is just under 107K across most of the Spanish-speaking countries as shown in the figure below.



Greater scientific productivity: *As well as speed increases, the optimisation of codes for the ARCHER machine will enable problems to be solved in less time using fewer compute resources.*

The Consortium has an active programme of software development. Developments in 2018-2019 included the following:

- MCC members and EPCC: MCC Flagship project (SAINT) is based around developing a webpage accessible database and software toolkit for surfaces and interfaces. This project is funded by EPSRC (EP/P022235, PI Scott Woodley) and supported by COSEC. The SAINT project has a number of key workpackages, which include developments to ChemShell, CP2K and automated calculations using CRYSTAL. For the latter, COSEC have provided support for expanding the range of elements that canbe included in our models.
- COSEC support: integration of DL_MONTE with ChemShell ; and an extensive testing suite created for DL_POLY in order to enhance program stability.
- Richard Catlow, Alexey Sokol, Thomas Keal: awarded EPSRC funding to extend ChemShell to model spectroscopic signatures with applications in nitrogen chemistry in catalysis and life sciences.
- Kostya Trachenko (QMUL): awarded an EPSRC Impact Acceleration Award (£46k) to develop DL_POLY by introducing the calculation of new properties (time correlation functions, elastic constants, current correlation functions etc), and has contracted Daresbury Laboratory to carry out this work.
- Arash Mostofi (IC): develops the ONETEP linear-scaling density-functional theory code (www.onetep.org). Held a ONETEP Masterclass in August 2019 at the University of Warwick for 30 participants, including from industry (AWE, Johnson Matthey).
- Jochen Blumberger (UCL): since the November 2018, has further improved and developed their inhouse fragment orbital-based surface hopping (FOB-SH) CP2K code for studying charge transport in large condensed phase systems. Code profiling and technical improvements have allowed to study transport across several thousands of atoms.
- Matthew Watkins (Lincoln): PAWing CP2K, an ARCHER funded eCSE project to include frozen core PAW functionality into CP2K.
- Steve Parker (Bath): Dr Tom Underwood is a developer of the general-purpose Monte Carlo simulation program DL_MONTE. Since November 2018 he has made many improvements to DL_MONTE. These include new features (liquid-crystal potentials; features to improve the general usability of the program), bug fixes, a new website, and the implementation of continuous integration and other practices to improve the sustainability of DL_MONTE. The number of registered DL_MONTE users has greatly increased since November 2018. The research has been exhibited at numerous UK conferences, and applying DL_MONTE to more challenging systems is the focus of a new PhD project in collaboration with AWE.
- Andrew Logsdail (Cardiff): Continued development of FHI-aims (SCF convergence for meta-GGAs and hybrids, including Pulay mixing) and Py-ChemShell (data structure management and tutorial content). This has no direct impact on consortium members other than group members, to my knowledge, but offers long-term capability for expansion of user bases.
- Aron Walsh (IC): The second version of the code SMACT (https://github.com/WMD-group/SMACT) has been release to facilitate screening of large chemical spaces.
- Aron Walsh (IC): The code CarrierCapture (https://github.com/WMD-group/CarrierCapture.jl) allows post-processing of DFT calculations to calculate carrier capture rates by defects in semiconductors and dielectrics.
- Clotilde Cucinotta (IC): Interfacing Smeagol and Cp2k – Initial stage. In progress (hired postdoc starting in January 2020)
- Chris Lorenz (KCL): developing software for the MDAnalysis software platform, which is open source and very popular within the classical MD community. Have contributed packages on calculating the survival probability of adsorption of one type of molecule around another molecule, and also some sophisticated analysis of the hydrogen bonding that occurs within aqueous environments.
- Chris Lorenz (KCL): Paul Smith and Mateusz Bieniek had been awarded the Warren L. DeLano Memorial PyMOL Open-Source Fellowship ($8000 for the year) for 2018-2019, and have made some significant enhancements of the PyMOL software package which again is commonly used by members of our community. These enhancements should start to percolate out into new releases code during the coming year.

- Clare Grey (Cambridge): Matt Evans, has been involved in developing the Matador package. This is an ongoing project in which Matt is adding extra functionality over time. Matador is a database for storing crystal structures (e.g. from structure searching calculations) and for carrying out associated calculations, e.g. voltage profiles or convex hulls.
- Ricardo Grau-Crespo (Reading): is involved in developing the SOD code (latest release, version 0.47, on 31st January 2019: https://github.com/gcmt-group/sod/releases/tag/0.47) for the simulation of solid solutions. It has been used in over 20 publications in the last year, mainly for the simulation of energy materials.
- Jonathan Skelton (Manchester): "Phonopy-Spectroscopy" for simulating IR/Raman spectra using Phonopy, which is being used by a number of research groups worldwide and has been integrated into a tool developed by the CNRS (France) to help inexperienced users work with modelling codes.
- Jonathan Skelton (Manchester): "Transformer" for enumerating symmetry-inequivalent atomic substitutions and generating solid-solution models, which is currently in the development stage but has already led to a paper in Chem. Mater.

Increasing the UK's CSE skills base (including graduate and post doctorate training and support):

During this reporting period, ~120 new ARCHER accounts on e05 were created, all of whom are new to our consortium and the majority of whom will have accessed ARCHER for the first time. Hence, the number of PhDs and Post-Docs that have been trained in the use of ARCHER as a result of work relating to the Consortium is ~120. If a breakdown between PhD and Post-Docs is required, please let us know.
Training activities include

- Consortium meetings, held every six months, typically include items on software development and during which best practice is shared and discussed. Software developments funded by the SIANT programme, our flagship project, is also disseminated during the morning session (oral presentations) of our meetings. MCC members and their group members are targeted; typically over 130 people attend our meetings.
- Consortium members are actively encouraged to attend workshops and training events organised by EPCC and STFC RAL and Daresbury.

Members also help run software workshops, for example:

- DL_MONTE workshop - to be held in Bath in January - to introduce prospective users of DL_MONTE and Monte Carlo simulation.
- ONETEP Masterclass – held in August 2019 at the University of Warwick for 30 participants, including from industry (AWE, Johnson Matthey). More details can be found on the Masterclass webpage: http://www.onetep.org/Main/MasterClass2019

It is also worth noting that during the last 12 months members have reported that 7 Master and 23 PhD students completed, and that several students trained by the consortium in applications of HPC techniques in Materials Chemistry have been recruited by Universities and Industry. Recent examples include an MRes graduate from UCL starting a PhD at KCL, PhD graduates also taking up a Post-doctoral position outside their original group in the UK (for example, went to Warwick, Queen Mary University of London), overseas (National University of Singapore; Harvard University; Kufa University, Iraq; NTNU Trondheim, Norway; Lawrence Berkeley National Laboratory, USA; Shenzhen Institute for Qunatum Science and Technology, Southern University of Science and Technology, China) or joining public bodies or private companies (CEA in France; Amazon; data analysis scientist at the Diamond Light Source; data scientist at Data&Data; programmer, MOD; BEIS, UK Government).
A number of Post-Docs have become lecturers or independent research fellows (for example, at Kings College London; Max Planck Institute for Structure and Dynamics of Matter, Hamburg; Institute of Physics and Biophysics, University of South Bohemia, Czech Republic; Center of Molecular and Macromolecular Studies, Lodz, Poland; Engineering, South Bank University), or moved to start a new Post-Doc position (in Sheffield; and in Glasglow), whereas other Post-Docs have, for example: become a Computational Scientist at STFC; research associate at Harwell; cofounded Nanolayers research computing; obtained a permanent appointment at the Turning Institute.

Increased impact and collaboration with industry: *ARCHER does not operate in isolation and the 'impact' of ARCHER's science is converted to economic growth through the interfaces with business and industry. In order to capture the impacts, which may be economic, social, environmental, scientific or political, various metrics may be utilised.*

Collaborations and Participation

The consortium has extensive and growing links with industry, members are also actively involved in panel and advisory groups with UK industry. The following are good examples:

- Nikolas Kaltsoyannis: work on the surface chemistry of the actinide dioxides, and in particular that being done by my student Jia-Li Chen using Archer, is in collaboration with Sellafield Limited. The work is of interest to them as it is helping to understand the possible mechanisms for the generation of gases within some of the canisters which store the UK's stockpile of civil plutonium, as PuO_2. The work forms part of the EPSRC's TRANSCEND nuclear waste and decommissioning consortium (https:// transcendconsortium.org/), a c. £10 M grouping of 11 university partners and multiple organisations from the nuclear industry.
- Alberto Roldan Martinez: JM gave support (£9k) for the First Grant which lead to a publication on cluster-support mismatch.
- Alex Shluger: Collaboration with Infineon Technologies Austria AG resulted in identification of recombination centres in 4H-SiC and at the 4H-SiC/SiO2 interface detected by electrically detected magnetic resonance and investigated using ab initio modelling performed on ARCHER. These defects are responsible for degradation in performance of SiC/SiO2 based devices and these results are used for improving the technology. These calculations were performed as a part of EngD studentship co-funded by Infineon, which provided £32K to UCL M3S CDT.
- Steve Parker: the study "Defect segregation facilitates oxygen transport at fluorite UO_2 grain boundaries", published in philosophical transactions A, was part of an industrial collaboration with AWE and was directly facilitated by MCC membership (use of Archer). Large scale molecular dynamics simulations were necessary to reliably investigate the diffusion paths. In addition, we have also been working with AWE towards understanding the aging of f-metal oxides. This included studying the adsorption of carbon dioxide on the surfaces of cerium oxide (Publication pending). In this instance, expensive density functional calculations have been utilised and would not have been possible without Archer.
- Aron Walsh: work performed on hybrid halide perovskites has led to a new collaboration with Samsung Research UK. This has led to a seed fund investment of £100k from Samsung to research at Imperial.
- Chris Lorenz (KCL): collaborated with NPL on some work related to the design of antimicrobial peptide nanocapsids. The simulations allowed them to understand the atomistic detail of the structures that were formed in their experiments, and in doing so provide a beginning to develop design rules for these nanocapsids.
- Graeme Day (Southampton): work with Pfizer and the Cambridge Crystallographic Data Centre supported a PhD student.

- Nikolas Kaltsoyannis: My team and I attend the meetings of the TRANSCEND consortium, as do Sellafield Limited and other nuclear industry partners. For example, the annual meeting of the full TRANSCEND consortium in Bath (April 2019) and the TRANSCEND Nuclear Materials Theme meeting at Lancaster (Nov 2019).
- Arash Mostofi: ONETEP Masterclass – held in August 2019 at the University of Warwick for 30 participants, including from industry (AWE, Johnson Matthey). More details can be found on the Masterclass webpage: http://www.onetep.org/Main/MasterClass2019
- Arash Mostofi: I have given two invited talks on work that was partly done using HPC time through the MCC. One at Continental in Hannover (8/10/19) and the other at Covestro in Leverkusen (13/9/19). Both were on theory and simulation of the mechanical properties of polymers and polymer nanocomposites.

- Steve Parker (Bath): applying DL_MONTE to more challenging systems is the focus of a new PhD project in collaboration with AWE.
- Clare Grey (Cambridge): Two of our members, Kent Griffith and Clare Grey, are major shareholders in a start-up company developing fast-charging batteries based on high-rate anode materials. See for example the acknowledgements section in 10.1021/jacs.9b06669.
- Keith McKenna (York): Two currently funded EPSRC projects have industrial involvement in an advisory capacity. These include: a project focused on improving the mobility of nanocrystalline TiO_2 (EP/P006051/1) involving Tronox Ltd (one of the worlds largest TiO_2 manufacturers, https://www.tronox.com) and a project focussed on computational screening on solar absorber materials for next generation photovoltaics (EP/P023843/1) involving Greatcell Energy (https://www.greatcellsolar.com). Both projects have led to publications acknowledging MCC and Archer.
- Graeme Day (Southampton): Membership of the Crystal Structure Prediction working group, hosted by the Cambridge Crystallographic Data Centre, involving industrial and academic partners.

Publications

From our Google form, the following 2018-19 papers were indicated as having industrial co-authors:

- Self-compensation in transparent conductor F-doped SnO_2, J. E. N. Swallow, B. A. D. Williamson, T. J. Whittles, A. Abbott, M. Farnworth, Kieran J. Cheetham, P. Warren, D. O. Scanlon, V. R. Dhanak, and T. D. Veal, *Adv. Funct. Mater*. 2018 **28** 1701900; http://dx.doi.org/10.1002/adfm.201701900
- HAXPES-Lab: A laboratory-based hard X-ray photoelectron spectrometer, A. Regoutz, P. Palmgren, S. K. Eriksson, M. Mascheck, C. Lijenberg, K. Tetzner, B. A. D. Williamson, D. O. Scanlon and T. Wiell, Rev. Sci. Inst. 2018 **89** 73105; http://dx.doi.org/10.1063/1.5039829
- A hard X-ray photoemission study of transparent conducting fluorine doped tin dioxide, J. E. N. Swallow, B. A. D. Williamson, M. Birkett, A. Abbott, M. Farnworth, T. J. Featherstone, N. Peng, P. Warren, A. Regoutz, D. A. Duncan, T.-L. Lee, D. O. Scanlon, R. R. Dhanak and T. D. Veal, *IEEE 7th World Conference on Photovoltaic Energy Conversion* 2018 **3** 3051; http://dx.doi.org/10.1109/PVSC.2018.8547950
- Low temperature ferroelectric behavior in morphotropic Pb $(Zr_{1-x}Ti_x)_{O-3}$, J. B. J. Chapman, O. T. Gindele, C. Vecchini, P. Thompson, M. Stewart, M. G. Cain, D. M. Duffy and A.V. Kimmel, *J. Amer. Ceram. Soc.* 2018 **101** 874-882; http://dx.doi.org/10.1111/jace.15101
- The critical role of hydrogen on the stability of oxy-hydroxyl defect clusters in uranium oxide, J. M. Flitcroft, M. Molinari, N. A. Brincat, N. R. Williams, M. T. Storr, G. C. Allen and S. C. Parker, *J. Mater. Chem. A* 2018 **6** 11362; http://dx.doi.org/10.1039/c8ta02817f
- Recombination defects at the 4H-SiC/SiO_2 interface investigated with electrically detected magnetic resonance and ab initio calculations, J. Cottom, G. Gruber, G. Pobegen, T. Aichinger, and A. L. Shluger, *J. App. Phys*. 2018 **124** 45302; http://dx.doi.org/10.1063/1.5024608
- Intrinsic electron trapping in amorphous oxides, J. Strand, M. Kaviani, V. V. Afanas'ev, J. G. Lisoni and A. L. Shluger, *Nanotech* 2018 **29** 125703; http://dx.doi.org/10.1088/1361-6528/aaa77a
- Hydrogen bonding versus entropy: revealing the underlying thermodynamics of the hybrid organic-inorganic Perovskite $[CH_3NH_3]PbBr_3$, G. Kieslich, J. M. Skelton, J. Armstrong, Y. Wu, F. Wei, K. L. Svane, A. Walsh and K. T. Butler, *Chemistry of Materials* 2018; http://dx.doi.org/10.1021/acs.chemmater.8b03164
- Acoustic phonon lifetimes limit thermal transport in methylammonium lead iodide, A. Gold-Parker, P. M. Gehring, J. M. Skelton, I. C. Smith, D. Parshall, J. M. Frost, H. I. Karunadasa, A. Walsh and M. F. Toney, *PNAS*, 2018 **115** (47) 11905-11910; http://dx.doi.org/10.1073/pnas.1812227115
- Stability and electronic properties of planar defects in quaternary I2-II-IV-VI4 semiconductors, J. Park, S. Kim and A. Walsh, *J. Appl. Phys*. 2018 **124** (16) 165705; http://dx.doi.org/10.1063/1.5053424
- Mechanistic Insights into selective oxidation of polyaromatic compounds using RICO chemistry, E. Nowicka, N. W. Hickey, M. Sankar, R. L. Jenkins, D. W. Knight, D. J. Willock, G. J. Hutchings, M. Francisco and S. H. Taylor, *Chemistry – A European Journal*, 2018 **24** 12359-12369; http://dx.doi.org/10.1002/chem.201800423
- Hybrid-DFT modeling of lattice and surface vacancies in MnO, A. J. Logsdail, C. A. Downing, T. W. Keal, P. Sherwood, A. A. Sokol and C. R. A. Catlow, *J. Phys. Chem. C*, 2019 **123** (13) 8133; http://dx.doi.org/10.1021/acs.jpcc.8b07846

- Impact of hydrogen on the intermediate oxygen clusters and diffusion in fluorite structured UO_{2+x}, J.M. Flitcroft, A.R. Symington, M. Molinari, N.A. Brincat, N.R. Williams, S.C. Parker, *Inorg. Chem.* 2019 **58** (6) 3774-3779; http://dx.doi.org/10.1021/acs.inorgchem.8b03317

Strengthening of UK's international position: *The impacts of ARCHER's science extend beyond national borders and most science is delivered through partnerships on a national or international level.*

Collaborations

The consortium has a very extensive range of international collaborations of which the following are typical:

- Mats Persson: The experimental group of Leonhard Grill, Department of Physical Chemistry, University of Graz, Austria Density functional calculation of the structure and energy barriers for the tautomerisation of a porphycene-like molecule on a metal surface studied by this group using scanning tunnelling microscopy.
- Kostya Trachenko: Collaboration with the International Atomic Energy Agency of the UN using the data produced on Archer.
- Reinhard Maurer: MCC HPC resources on ARCHER have been used in a long-standing collaboration on machine learning methods in gas-surface dynamics simulations with colleagues at USTC, Hefei, China which led to three publications. Training data has been generated and simulations have been performed on ARCHER.
- Reinhard Maurer: MCC HPC resources on ARCHER have been used to simulate core-level spectroscopy within a joint experiment/theory international collaboration led by German partners.
- Members of the consortium (Shluger, Slater, Zwijnenburg, Walsh, Scanlon): are involved in the EPSRC grant Ref: EP/R034540/1 "Defect Functionalized Sustainable Energy Materials: From Design to Devices Application" which co-funds the collaboration within the EPSRC-JSPS Core-to-Core Collaboration in Advanced Materials and involves Tokyo Institute of Technology and several other institutions in Japan as well as the McGill University in Montreal, Canada.
- Sanliang Ling: In collaboration with colleagues from Sandia National Laboratories in the US, has started a new project on computational discovery of new hydrogen storage materials. The computer time on ARCHER enabled us to perform density functional theory calculations on a range of candidate materials for their potential application on solid-state hydrogen storage.
- Sanliang Ling: In collaboration with colleagues from South China University of Technology in China, has started a joint project on experimental synthesis of single atom catalyst on carbon materials and computational investigation of the electronic structures of these materials for energy-related applications.
- Jochen Blumberger: First principles molecular dynamics simulation of the hematite/water interface, in collaboration with Kevin Rosso at Pacific Northwest National Laboratory, US.
- Matthew Watkins: Ongoing collaborative research on nanolayers between University of Lincoln and a consortium of French experimental groups - lead by Christian Loppacher, Univeristy of Marseilles.
- Matthew Watkins: Collaboration with the CP2K development group - including international workshops and summer schools as well as code development and planning.
- Natalia Martsinovich: Collaboration with Dr M. Lackinger (Munich) on "Molecular self-assembly on surfaces" . Calculations of self-assembled molecular structures on metal surfaces used THOMAS.
- Andrew Logsdail: Development of FHI-aims remains an international collaboration (Duke, FHI, Munich), and the ARCHER/MCC Consortium allows the testing of this software on a state-of-the-art infrastructure.
- Aron Walsh: Research was performed as part of the EU consortium http://www.starcell.eu on kesterite solar cells. Computations were used to support experimental activities with partners in Germany, Sweden and Spain.
- Lev Kantorovich: Collaboration with the group of Prof. Angelika Kuhnle, Mainz University (Germany), where we revealed a complex kinetic mechanism governing a transformation of one self-assembled structure into the other. ARCHER played a vital role in calculating necessary reaction barrier (around 50

were calculated); without their knowledge it would have been impossible to understand the complex transformation mechanism at play.

- Lev Kantorovich: Collaboration with the group of Prof. J. M. Recio, Oviedo University (Spain). ARCHER was essential here for running simulations to uncover the walking mechanism of the molecule on the copper surface.
- John Harding: work has been done as a member of a programme grant (EP/R018820/; Crystallisation in the Real World: Delivering Control through Theory and Experiment) which involves both international collaboration (Jim DeYoreo (PNNL, USA) and Susan Stipp (Copenhagen) and Julian Gale (Curtin, Australia)) and industrial partners (Lubrizol Ltd; BP Exploration Operating Company Limited; Procter and Gamble). Computer time on ARCHER provided by MCC provided background evidence for proof of concept of the proposal.
- Johannes Lischner: collaboration with Weber-Bargioni group at Lawrence Berkeley Lab: ARCHER was used to calculate the properties of charged defects in transition-metal dichalcogenide monolayers. The results were in excellent agreement with experimental scanning tunnelling microscopy experiments carried out at Berkeley.
- Johannes Lischner: collaboration with Cho group in Seoul: ARCHER was used to calculated the electronic structure of heterostructures consisting of multilayer graphene and tantalum disulfide for novel spin-to-charge and charge-to-spin conversion devices. The results were used to underpin experimental transport measurements by Cho group in Korea.
- Chris Lorenz: simulation work on tetronic polymeric self-assembly is done in collaboration with experimentalists from King's and from Spain. Here are simulations have demonstrated a very unique perspective in the charge state of the polymers in solution, which previously had not been considered by the experimentalists, and therefore will provide a new understanding of the self-assembly process and the structures that result.
- Chris Lorenz: the structure and aggregation of the proteins that make up spider silk before they are extruded is being studied in collaboration with an experimental group in the USA and another simulation group in Paris, France. This is the first work of its kind and it will provide us with a true understanding of how the proteins transition from their amorphous structure inside the spider to the more ordered silk that is formed when it is extruded.
- Chris Lorenz: have used Archer computer time to investigate the effect of slight assymetry in the surface density of CTAB surfactants on the structure and dynamics of confined water. In doing so, we have been able to elucidate atomistic details of the cause of the assymetrical response observed experimentally by our experimental collaborators in the USA.
- Sarah (Sally) Price: Magnapharm is a EU-funded project involving our group at UCL and three experimental groups at University of Bristol, Radboud University Nijmegen, the Netherlands, and University of Limerick, Ireland. For our part in the project, we use ARCHER time allocated through the MCC consortium to calculate thermodynamic and magnetic properties of experimental or CSP-predicted crystal structures, which are then used to predict/interpret experimental observations of crystallizations in magnetic fields.
- Clare Grey: projects have involved international collaboration, e.g. 10.1021/jacs.9b06669 (in this case involving collaboration with researchers at the University of California and the University of Texas at Austin). In this case the collaboration related to experimental work, and resources provided by the MCC allowed calculations to be carried out to rationalise experimental results.
- Keith McKenna: collaboration with Verónica Salgueiriño (Universidade de Vigo, Vigo, Spain) on Antiphase boundaries in truncated Zn-doped magnetite nanocrystals.
- Keith McKenna: collaboration with Hannes Jónsson (University of Iceland, Iceland) and Yuichi Ikuhara (University of Tokyo, Japan) on the structure and properties of an edge dislocation in rutile TiO_2
- Keith McKenna: collaboration with Leopoldo Molina-Luna and Lambert Alff (Universität Darmstadt, Germany) on the structure and properties of grain boundaries in HfO_2-based resistive switching memory devices.
- Arunabhiram Chutia: collaboration with Dr. Alberto Villa (University of Milan), Dr. Peter P. Wells (University of Southampton) and Dr. Nikolaos Dimitratos (University of Bologna) on the interaction of furfural on Pd, NiO and TiO_2. To investigate the unique electronic properties of furfural interacting on

Pd, NiO and TiO_2 surfaces, calculations are performed using ARCHER and on HPC Midlands Plus.

- Arunabhiram Chutia: collaboration with Dr. Ikutaro Hamada (University of Osaka), Prof. Stewart F. Parker and Dr. Ian P. Silverwood (STFC) on the interaction of catalytically interesting molecule on Ni(h,k,l) surface. All the DFT based quantum chemical calculations for this project is performed on ARCHER and on HPC Midlands Plus.
- Graeme Day: collaboration with Lyndon Emsley (EPFL, Switzerland), using ARCHER for developing methods for NMR crystallography.
- Graeme Day: collaboration with Michelle Ceriotti (EPFL, Switzerland), using ARCHER for generating date used in machine learning of crystal structure landscapes and properties.
- Graeme Day: collaboration with Gregory Beran (UC Riverside, USA), using ARCHER for benchmarking methods for NMR chemical shift prediction.
- Graeme Day: collaboration with Erin Johnson (Dalhousie, Canada), using ARCHER for generating data for benchmarking errors in DFT calculations on molecular crystals.
- Ricardo Grau-Crespo: collaboration with the group of Prof. Francesc Illas (University of Barcelona, Spain) led to paper "Double-well potential energy surface in the interaction between h-BN and Ni (111)", by J Ontaneda, F Viñes, F Illas, R Grau-Crespo. Physical Chemistry Chemical Physics 21 (2019), 10888-10894. Calculations performed in ARCHER with time distributed by the MCC.
- Ricardo Grau-Crespo: collaboration with the group of Prof. Udo Schwingenschlögl (KAUST, Saudi Arabia) led to paper "Origin of the transition entropy in vanadium dioxide" by TA Mellan, H Wang, U Schwingenschlögl, R Grau-Crespo. Physical Review B 99 (2019), 064113. Calculations performed in ARCHER with time distributed by the MCC.
- Jonathan Skelton: modelling polarised Raman spectra with collaborators in NUI Galway (Ireland).
- Jonathan Skelton: modelling structural flexibility in MOFs with collaborators in Technical University of Munich (Germany).
- Jonathan Skelton: modelling conductive MOFs with collaborators in University of Southern California (US).

Publications

From our Google form, the following 2018 and 2019 papers were indicated as having international based co-authors:

- Recombination defects at the 4H-SiC/SiO2 interface investigated with electrically detected magnetic resonance and ab initio calculations, J. Cottom, G. Gruber, G. Pobegen, T. Aichinger, and A. L. Shluger, *Jour. App. Phys.* 2018 **124** 45302; http://dx.doi.org/10.1063/1.5024608
- Synthesis, crystal structure, magnetic and electronic properties of the caesium-based transition metal halide $Cs_3Fe_2Br_9$, Fengxia Wei, Federico Brivio, Yue Wu, Shijing Sun, Paul D. Bristowe and Anthony K. Cheetham, *J. Mat. Chem. C* 2018; http://dx.doi.org/10.1039/c7tc04798c
- Reactivity of CO_2 on the surfaces of magnetite (Fe_3O_4), greigite (Fe_3S_4) and mackinawite (FeS), D. Santos-Carballal, A. Roldan, N.Y. Dzade, N.H. de Leeuw, *Philos. Trans. R. Soc. A Math. Phys. Eng. Sci*. 2018 **376** (2110) 20170065; http://dx.doi.org/10.1098/rsta.2017.0065
- Density functional study of carbon vacancies in titanium carbide, M. Råsander, H. W. Hugosson and A. Delin, *J. Phys. Condens Matter* 2018 **30** 15702; http://dx.doi.org/10.1088/1361-648X/aa9979
- Water Participation in Catalysis: An Atomistic Approach to Solvent Effects in the Catalytic Isomerization of Allylic Alcohols, F. Scalambra, N. Holzmann, L. Bernasconi, S. Imberti, A. Romerosa, *ACS Catal*. 2018 **8** (5) 3812-3819; http://dx.doi.org/10.1021/acscatal.8b00199
- Anharmonicity and Octahedral Tilting in Defect-Ordered Hybrid Perovskites, A. E. Maughan, A. M. Ganose, A. M. Canadia, J. T. Granger, D. O. Scanlon, and J. R. Neilson, *Chem. Mater*. 2018 **30** 472; http://dx.doi.org/10.1021/acs.chemmater.7b04516
- Deeper Understanding of Interstitial Boron-Doped Anatase Thin Films as A Multifunctional Layer Through Theory and Experiment, M. Quesada-Gonzalez, B. A. D. Williamson, C. Sotelo-Vasquez, A. Kafizas, N. D. Boscher, R. Quesada-Cabrera, D. O. Scanlon, C. J. Carmalt, and I. P. Parkin, *J. Phys. Chem. C* 2018 **122** 714; http://dx.doi.org/10.1021/acs.jpcc.7b11142
- Local corrugation and persistent charge density wave in $ZrTe_3$ with Ni intercalation, A. M. Ganose, L. Gannon, F. Babrizi, H, Nowell, S. Barnett, H. Lei, X. Zhu, C. Pertovic, D. O. Scanlon and M. Hoesch, *Phys.*

Rev. B 2018 **97** 155103; http://dx.doi.org/10.1103/PhysRevB.97.155103
- First-Principles Insights into Tin-Based Two-Dimensional Hybrid Halide Perovskites for Photovoltaics, Z. Wang, A. M. Ganose, C. Niu, and D. O. Scanlon, *J. Mater. Chem. A*, 2018 5652; http://dx.doi.org/10.1039/C8TA00751A
- Band gap temperature-dependence and exciton-like state in copper antimony sulphide, $CuSbS_2$, M. Birkett, C. N. Savory, M. K. Rajpalke, W. M. Linhart, T. J. Whittles, J. T. Gibbon, A. W. Welch, I. Z. Mitrovic, A. Zakutayev, D. O. Scanlon, and T. D. Veal, *APL Mater.* 2018 **6** 84904; http://dx.doi.org/10.1063/1.5030207
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Participation

The work of the consortium has received considerable international attention, with members invited to present their work at major international conferences. Here we provide a list of international talks from two established members and one new member of the consortium:

- Lev Kantorovich gave an invited talk at the Advanced Problems in Mechanics, the XLVII International Summer School-Conference, St. Petersburg, Russia, June 24-29 2019.
- Alex Shluger gave invited talks at: Insulating Films on Semiconductors (INFOS2019); Fall meeting of E-MRS; International Conference on Memristive Materials, Devices & Systems (MEMRISYS 2019); International Workshop on Characterization and Modelling of Memory Devices, Milano 2019; International Workshop on Computational Nanotechnology, Orrington 2019; XXVIII International Materials Research Congress, Cancun 2019; Towards Reality in Nanoscale Materials X, Levi 2019; RRAM/MRAM Workshop, Leuven 2019.
- Clotilde Cucinotta: 21-22 October 2019, Third International Computational Science and Engineering Conference ICSEC19. Qatar, Tamu, EDU, Invited Seminar: Improving the design of materials and electrochemical devices for energy and nanotechnology using theory and modelling.

Other Highlights for the Current Reporting Period: Please provide details of any other significant highlights from the reporting period that are not captured elsewhere in the report.

NA

HEC Consortia Model: Over the coming months EPSRC will be looking at the future of the HEC Consortia model and potential future funding. We would like to use this opportunity to ask the Consortia Chairs for input:

The consortium model continues to be of substantial benefit to the materials modelling community and has indeed played a major role in ensuring the UK science remains at the forefront in this field. The benefits of the model include:

- Ensuring that members have access to state-of-the-art software.
- Promoting the most effective and efficient usage of HEC resources.
- Facilitation of collaboration and interaction between members in both software development and applications.
- Provision of a focal point for UK science in the field, thereby assisting international collaborations.
- Promotion of the broader impact and development of industrial usage of HEC.
- Effective dissemination and outreach for HEC in materials science.
- Provides transparency and accountability of access and allocation of UK resources

The consortium has effective support from the COSEC.

Web-Content Approval:

Please indicate which sections of the annual report could be used to produce content for the Consortia pages on the ARCHER website: https://www.archer.ac.uk/community/consortia/

Section Heading	Yes / No / Maybe	Comments
Membership	Yes to committee (theme leaders), Maybe to list all other members	
World class and world leading scientific output	Yes	
Greater scientific productivity:	Yes	
Increasing the UK's CSE skills base	Yes	
Increased impact and collaboration with industry	Yes	
Strengthening of UK's international position**:**	Yes	
Other Highlights for the Current Reporting Period	Yes	

To Note: New web-content generated from the annual reports will not be published without the approval of the relevant Consortium Chair.