



University of  
**Strathclyde**  
Glasgow



Royal Charter  
since 1964  
Useful Learning  
since 1796



# Research Fellow/Associate in Computational Chemistry

Department	Pure and Applied Chemistry ( <a href="http://www.strath.ac.uk/science/chemistry/">www.strath.ac.uk/science/chemistry/</a> )		
Faculty	Faculty of Science ( <a href="http://www.strath.ac.uk/science/">www.strath.ac.uk/science/</a> )		
Staff Category	Research	Reference No	611015
Reports To	Head of Department, through Dr David Nelson	Grade	*8
Salary Range	£45585	Contract Type	Fixed Term (36 months)
FTE	1.0 A part-time appointment may be possible.	Closing Date	07/06/2024
Holidays	31 days + 11 statutory days Option to purchase additional holidays.	On Site Facilities	Car parking, sports centre, catering.
Pensions	Contributory pension scheme available to all staff including generous employer contribution.		
Training	Professional Development with <a href="#">Organisational and Staff Development Unit</a> (OSDU) plus external training if required.		
Family Friendly Benefits	Generous parental leave provision, on-campus nursery and options for flexible working.		
Health and Wellbeing	University Sport centre, Occupational Health service, access to health and wellbeing events, cycle to work scheme, Employee Assistance Programme, agile working and established carers support network and carer friendly policies.		

## Job Advert

A computational chemistry researcher is required to deliver an ambitious research programme to understand reaction mechanisms in homogeneous catalysis by complexes of nickel, generously funded by the Leverhulme Trust for three years. The position is nominally 1 FTE, but it may be possible to offer this on a part-time basis and/or with some component of hybrid working; the position will not be offered on a fully remote basis.

We have studied the reactions of homogeneous nickel(0) complexes with a variety of organic substrates in some detail (*Catal. Sci. Technol.*, 2021, **11**, 2980). Nickel(0) can react with organohalides *via* mechanisms including oxidative addition, halogen atom abstraction, and electron transfer, and it possible that spin crossover plays a role in some cases. The exact mechanism(s) that operate are highly dependent on the nature of the ligand and the substrate in each specific reaction. This project will assess the fundamental features of each system that influence reaction selectivity, with the aim of producing a unified model that can predict the reactivity of any nickel catalyst system. While the research team is primarily focused on laboratory experimental studies, the use of computational chemistry is becoming increasingly important to deliver our research objectives, and you will be the computational chemistry expert within the team. The project will be carried out using the ARCHIE-WeSt High-Performance Computer hosted at the University of Strathclyde ([archie-west.ac.uk](http://archie-west.ac.uk)), which comprises 84 'standard' nodes (40 cores, 192 GB RAM), two 'bigmem' nodes (80 cores, 3 TB RAM), and 24 Nvidia A100 GPUs (8 x 40 GB; 16 x 80 GB). High priority access is costed into the project.

You will engage in individual and collaborative research, establishing a distinctive programme of research and disseminating results through regular publications in high impact journals. You will mentor and support junior researchers within the team,

### the place of useful learning

The University of Strathclyde is a charitable body, registered in Scotland, number SC015263

including MChem and PhD students carrying out computational chemistry projects. You will contribute to applications to appropriate external bodies for research funding. You will provide direction, support and guidance to team members and you will participate in and develop external networks to foster research collaborations, to inform the development of research objectives and to identify potential sources of funding. You will develop knowledge exchange activities by, for example, establishing research links with industry, and you will collaborate with colleagues to ensure that research advances inform departmental teaching effort, including contributing to relevant teaching programmes as appropriate. You will carry out Department/School, Faculty and/or University administrative and management functions, for example through membership of committees and engage in continuous professional development. It is possible to undertake a Postgraduate Certificate or Postgraduate Diploma in Academic Practice or Researcher Development, at no cost, in parallel with your position.

To be considered for the role, you will be educated to a minimum of PhD level in an appropriate discipline or have significant relevant experience in addition to a relevant degree. You will have sufficient breadth and depth of expertise and experience in computational chemistry as applied to homogeneous catalysis, as well as the fundamental principles of organometallic chemistry and organometallic reaction mechanisms.

You will have significant research experience in computational chemistry applied to homogeneous catalysis and in the practical use of machine learning or other relevant statistical techniques to interrogate large datasets and make predictions. Postdoctoral experience would be a significant advantage. You will have a body of published high quality research demonstrating standards of excellence, and an ability to develop research proposals and to attract funding, as appropriate to the discipline, including experience of contributing to grant applications. You will have an ability to plan and organise research programmes, to ensure successful completion and you will have experience of planning and organising workloads, including the ability to supervise and delegate work. You may have some experience of teaching at undergraduate and/or postgraduate levels and will have an ability to work within a team environment and to lead teams.

You will have excellent interpersonal and communication skills, with the ability to listen, engage and persuade, and to present complex information in an accessible way to a range of audiences. Whilst not essential for the role, applications are welcomed from candidates with membership of relevant Chartered/professional bodies (including the Higher Education Academy, the Royal Society of Chemistry, and/or the American Chemical Society) and/or a track record in knowledge exchange related activities.

\*Whilst a Research Fellow is ideally sought for the position, applications from less-experienced Researchers are welcomed. In such circumstances, the appointment will be made at Research Associate level (RS07 salary scale: £36,024 - £44,263) and duties will be adjusted to reflect the grade of the post.

Please note that any appointment to this position is subject to the approval of the Leverhulme Trust and that a copy of your CV will require to be shared with the Trust before employment can commence.

## Job Description

### Brief Outline of Job:

To pursue and establish a high quality research programme, including securing research contracts and funding; to disseminate research results via publications in peer reviewed journals; where appropriate, to manage a research team; and to engage as appropriate in relevant teaching, professional and knowledge exchange activities.

### Main Activities/Responsibilities:

1.	Engage as a researcher in individual and collaborative research, establishing a distinctive programme of research and disseminating results through regular high impact publications in journals.
2.	Support or submit applications for external funding, as Co-I or PI where appropriate
3.	Manage a research team, providing direction, support and guidance in your areas of specialism.
4.	Participate in and develop external networks to foster research collaborations, to inform the development of research objectives and to identify potential sources of funding.
5.	Develop knowledge exchange activities by, for example, establishing research links with industry and/or other academic research teams.
6.	Collaborate with colleagues to ensure that research advances inform departmental teaching effort, including contributing to relevant teaching programmes as appropriate.
7.	Carry out Department, Faculty and/or University administrative and management functions, for example through membership of committees, as agreed with your line manager
8.	Engage in continuous professional development.

## Person Specification

### Educational and/or Professional Qualifications

(E=Essential, i.e. a candidate must meet all essential criteria to be considered for selection, D=Desirable)

E1 Good honours degree and PhD (or, exceptionally, equivalent professional experience) in appropriate discipline.

D1 Membership of relevant Chartered/professional bodies (including Higher Education Academy).

### Experience

D2 Some experience of teaching at undergraduate and/or postgraduate levels, and/or mentoring and supporting junior researchers within a team.

E2 Experience of planning and organising workload, including the ability to supervise and delegate work.

E3 Experience of computational chemistry applied to understanding homogeneous catalysis.

D3 Experience of applying machine learning or other statistical classification or regression methods to gain deeper insight from large datasets.

E4 Good fundamental knowledge of organometallic chemistry and catalysis by transition metals.

### Job Related Skills and Achievements

E5 A body of published high quality research publications demonstrating standards of excellence.

D4 Ability to develop research proposals and to attract funding, as appropriate to the discipline, including experience of contributing to grant applications.

E6 Ability to plan and organise research programmes to ensure successful completion.

E7 Ability to work within a team environment and to lead teams.

D5 Track record in knowledge exchange related activities.

### Personal Attributes

E8 Excellent interpersonal and communication skills, with the ability to listen, engage and persuade, and to present complex information in an accessible way to a range of audiences.

E9 Research interests in the broad fields of computational chemistry applied to transition metal catalysis.

## Application Procedure

Applicants are required to complete an application form including the name of three referees who will be contacted without further permission, unless you indicate that you would prefer otherwise. Applicants should also submit a Curriculum Vitae and a covering letter detailing the knowledge, skills and experience you think make you the right candidate for the job. Applicants should also complete the Equal Opportunities Monitoring Form.

## Other Information

Further information on the application process and working at Strathclyde can be found on our website

(<http://www.strath.ac.uk/hr/workforum>).

Informal enquiries about the post can be directed to Dr David Nelson, Reader in Chemistry ([david.nelson@strath.ac.uk](mailto:david.nelson@strath.ac.uk)).

Applications cannot be accepted *via* email and must be submitted *via* the University of Strathclyde website to be considered.

### Conditions of Employment

Conditions of employment relating to the Research staff category can be found at: [Conditions of Employment](#).

### Rewards and Benefits

Our staff have access to a wide range of outstanding benefits that include financial rewards, family friendly and wellbeing benefits and career development opportunities, details of which can be found [here](#).

### Pre-employment health screening

An offer of appointment will be subject to a medical assessment by Occupational Health. An individual who accepts an offer of employment must complete a confidential medical questionnaire and forward it to the Occupational Health Nurse within 5

days of receipt. If further information is required the individual may be contacted by the OHN or a Medical Advisor and a personal appointment with the individual may be arranged. An unconditional contract of employment will not be issued until Human Resources receives confirmation that applicant is fit to undertake the duties of the post.

### Probation

Where applicable, the successful applicant will be required to serve a 12 month probationary period.

### Pension

The successful applicant will be eligible to join the Universities' Superannuation Scheme. Further information regarding this scheme is available from [Payroll and Pensions](#).

### Relocation

Where applicable, the University offers a relocation package to support new employees who meet the eligibility criteria. The relocation package is offered as a contribution towards costs incurred, and is designed to be flexible, allowing staff to use the financial support available in the way that will be most helpful to them. Further details are outlined in the Relocation Policy.

### Interviews

Formal interviews for this post will be held on Monday, 8 July 2024 between 10 am and 4 pm.

### Equality and Diversity

The University of Strathclyde is a socially progressive institution that strives to ensure equality of opportunity and celebrates the diversity of its student and staff community. Strathclyde is people-oriented and collaborative, offering a supportive and flexible working culture with a deep commitment to our equality, diversity and inclusion charters, initiatives, groups and networks.

We strongly encourage applications from Black, Asian and minority ethnicity, women, LGBT+, and disabled candidates and candidates from lower socio-economic groups and care-experienced backgrounds.

### University Values

The University's Values capture what we're all about: who we are, what we believe in and what we stand for. [Our Values](#) have been derived from how we act and how we expect to be treated as part of Strathclyde.



# Conditions of Employment

## Research Staff

### 1. GENERAL CONDITIONS

Members of staff are subject to the Charter and Statutes and the Ordinances and Regulations of the University, published in the Calendar, and to any amendments or additions thereto approved by the University Court and, in the case of the Charter and Statutes, the Privy Council. Staff are also expected to familiarise themselves with, and adhere to, general University policies and procedures, as published on University web pages.

The University Court recognises Strathclyde Universities and College Union (SUCU) as the sole body with which it will negotiate and consult on all collective issues concerned with the terms and conditions of employment of Research Staff. Such terms and conditions may be varied by the University Court after negotiation and consultation with SUCU.

Each member of staff is responsible for the proper performance of allocated duties to the person or persons specified in the member of staff's letter of appointment and any accompanying papers.

The University is committed to ensuring that its business is conducted in an open and transparent manner and will take all appropriate steps to address risks of bribery or corruption. Members of staff are required at all times to act honestly and with integrity and to safeguard the resources for which they are responsible. The University has in place a robust Public Interest Disclosure (Whistleblowing) Policy to enable concerns to be brought to its attention. This is available at [www.strath.ac.uk/publicinterestdisclosure](http://www.strath.ac.uk/publicinterestdisclosure). Other relevant policies, e.g. Fraud Prevention and Conflicts of Interests, can also be found on the University's website.

Any member of staff may at any time be exposed to commercially sensitive information, information related to potentially valuable intellectual property or information which may otherwise be of a confidential nature. This information, which could be found anywhere in the University, may be written or disclosed orally, can include information of a commercial or technical nature, and may be owned by the University or by third parties. The University requires all employees to keep any such information confidential in the first instance and not disclose, publish or otherwise disseminate it without prior consent of the University. Such confidentiality obligations are commonplace and in the commercial interests of the University. When in doubt advice should always be sought from Research and Knowledge Exchange Services prior to disclosure.

The University operates probationary periods for new staff, the duration of which will be specified in individual letters of appointment. The normal probation period for posts in this staff category is 9 months for those at grades 6 and 7, and 12 months for grades 8 and above. Further guidance on probationary procedures is published at <http://www.strath.ac.uk/staff/policies/hr/>.

Further guidance on probationary procedures is published at [www.strath.ac.uk/hr](http://www.strath.ac.uk/hr).

Further information on the terms and conditions specified in this document and other staffing policies and procedures can also be found at [www.strath.ac.uk/hr](http://www.strath.ac.uk/hr).

### 2. SALARY

Appointments are made at an appropriate salary point on the University's grading structure, with initial placing determined according to qualifications and experience. Increments are paid to staff on the 12 month anniversary of their appointment. Where this is not the first of the month, the increment will be paid on the first of the month directly

after the 12 month anniversary. This allows 1 progression to the next point on the salary scale until the top guaranteed point of the scale is reached.

Salaries are paid directly to staff members nominated bank account, normally on the second last working day of the month.

### 3. HOURS OF WORK

Working time is that required to fulfil the duties of the post. The University Court recognises that research staff carry out these duties in a variety of ways appropriate to the nature of the research activity, but expects regular contact to take place between the research staff employee and the supervisor/granholder (where these positions are occupied by different individuals) during normal working hours on week days. There are exceptions to this pattern which may involve contact at other locations or in the evenings, or at weekends, but these arrangement will be made with the agreement of the member of staff concerned.

Duties may, by arrangement with Head of Department/School/Director, include some teaching associated with the post (up to a maximum of 40 hours per semester) for which no additional payment will be made.

Additional work which does not fall within the scope of that described above may by arrangement attract payment which must be authorised and processed through the payroll.

### 4. HOLIDAYS

Annual leave entitlement is 31 days per year to be taken by agreement with the line manager. For staff members working on a part-time basis, holidays will be calculated on a pro-rata basis.

In addition to annual leave there is an entitlement to eleven public holidays per year which should be taken on days that the University is closed for this purpose. The University presently closes for four additional days over the Christmas and New Year period. **These additional days count against the annual leave entitlement.**

For staff members working on a part-time basis, public holiday entitlement will be calculated on a pro-rata basis.

Annual leave and public holiday entitlements should be taken in the leave year to which they relate. Up to five days leave can be carried forward into the new leave year subject to line management agreement. In exceptional circumstances, Heads of Department/School/Director may approve carry forward of accrued annual leave in excess of five days.

The University's expectation is that staff take all accrued holidays prior to their termination date. If staff have exceeded their entitlement the University will deduct an equivalent number of days pay from final salary payments.



## 5. SICKNESS ABSENCE

During any period of absence through illness or injury provided the appropriate notification and certification procedures have been followed the University will pay a member of staff (having taken account of the aggregate of all periods of absence due to illness during the twelve months immediately preceding the first day of the current absence) as follows:

<b>Period of Continuous Employment at start of absence from work</b>	<b>Full Pay</b>	<b>Half Pay</b>
Less than 1 year	1 month	1 month
1 year but less than 2 years	2 months	2 months
2 years but less than 3 years	4 months	4 months
3 years but less than 5 years	5 months	5 months
5 years or more	6 months	6 months

In order to manage the University's sick pay scheme the University requires to maintain sickness absence records on individual members of staff. When making payments after the expiry of statutory sick pay the University will deduct an amount equivalent to any benefit normally payable by the Department of Work and Pensions. For full details on the general University policy in this area please refer to the Sickness Absence Management Policy at [www.strath.ac.uk/staff/policies/hr](http://www.strath.ac.uk/staff/policies/hr).

## 6. PENSIONS

If you are under age 75 at the date your appointment commences you will automatically become a member of the pension scheme operated by the University — the Universities Superannuation Scheme (USS). You will be admitted to the career revalued benefits scheme called the USS Retirement Income Builder; the contribution rate that currently applies is 6.1% of pensionable salary. A threshold applies to the maximum salary that counts towards the USS Retirement Income Builder. The current threshold from 1 April 2024 is £70,296 per year. Contributions based on salary above the monthly equivalent rate of the threshold are paid to the defined contribution section of the scheme called the USS Investment Builder. Please use the following link to access information, including the USS Member Guide: <https://www.uss.co.uk/for-members/youre-a-new-joiner>. The scheme booklet is called 'Your Guide to the Universities Superannuation Scheme'.

The University operates a salary exchange arrangement, Pensions Plus, for members of the USS. Pensions Plus enables pension contributions to be made in a manner so that both employees and the University can benefit from available National Insurance Contribution savings. You will be automatically included in Pensions Plus, provided it does not adversely affect your take-home pay or your ability to claim certain state benefits. If your earnings fall below the Pension Plus pay protection limit you will be opted out of Pension Plus. This will not affect your membership of the USS.

New members of staff may opt out of USS within three months of taking up appointment and will then be treated as if they had never been a member of the scheme. After three months members of staff who wish to withdraw from USS during their employment will be required to give a minimum of 28 days' notice in writing to the University. Any member of staff who wishes to opt out should contact the Pensions Section, Finance, in the first instance ([pensions@strath.ac.uk](mailto:pensions@strath.ac.uk)). Please note that if you are a member of Pensions Plus and withdraw from USS with less than two years of membership, or cease employment with the University and have less than two years of USS membership, the option of a refund of pension contributions will not be available to you. Instead, USS must provide you with a pension benefit that is payable from your Normal Pension Age. Regardless of whether you participate in Pensions Plus, if you are a member of the pension scheme for two years or more you are not entitled to a refund of pension contributions on leaving the scheme, you will be entitled to a pension benefit.

The University reserves the right to alter or withdraw Pensions Plus as it sees fit or as required to comply with legislative changes. Withdrawal or amendment of Pensions Plus will not affect your membership of USS. If you do not wish to participate in Pensions Plus but wish to remain in

the pension scheme please contact the Pensions Team who will provide you with a non-participation form.

Information regarding pension scheme membership can be found on the Pensions pages of the University's website. Full information regarding USS can be found on the USS website – [www.uss.co.uk](http://www.uss.co.uk)

## 7. PLACE OF WORK AND RESIDENCE

Members of staff will be based on the John Anderson Campus, unless otherwise stated in the letter of appointment. The Department/School in which the post is initially placed will be specified in the letter of appointment although there will be an expectation to work at such other places as required in the course of employment.

If the need arises for members of staff to work outside the UK for a period (or periods) of more than one month then such arrangements will be subject to mutual agreement. Members of staff would then be provided with a statement in advance setting out the terms covering such periods of employment.

The University does not normally place specific restrictions upon the place of residence of members of staff. All staff are, however, expected to reside in a location which is compatible with the satisfactory fulfilment of all the duties associated with their appointment.

## 8. CONSULTANCY/FURTHER ACTIVITIES

To support the strategic objectives of the University and to facilitate individual professional development, the University encourages staff to engage in professional activities with outside bodies related to their field of work. In many cases, such activity will be approved on the basis that it represents University knowledge exchange activity and should therefore be treated as part of the individual's overall workload and managed through the University's systems. It is also recognised that there will be some cases where an activity is entirely separate from the University and should thus be notified/approved as a personal business activity. For further information please refer to the "University Procedure in relation to Work for Outside Bodies including Consultancies", which forms part of the employment contract and can be accessed at [www.strath.ac.uk/hr](http://www.strath.ac.uk/hr).

## 9. DISCIPLINARY AND GRIEVANCE PROCEDURES

Further information on the University's disciplinary and grievance procedure can also be found at [www.strath.ac.uk/policies/hr](http://www.strath.ac.uk/policies/hr) or on request from Human Resources.

## 10. NOTICE AND TERMINATION

Members of staff are employed on the conditions indicated in individual letters of appointment and any accompanying papers. The University is not obliged to give notice of termination or continue any employment beyond the end of that period. Where the period of the contract of employment is for one year or less it may be terminated short of the fixed term period by one months notice on either side. Where the period of the contract of employment is for more than one year, or where there have been a further contract or series of contracts immediately consecutive, the employment may be terminated short of the fixed term period by three months' notice on either side, except during the probationary period when the notice period is one month.

If the appointment is for a fixed term it will expire at the end of the period without the necessity for notice.

Revised April 2024