CoreShell Molecular Descriptor PDRA (845552)

Faculty	Faculty of Science		
Department	Pure and Applied Chemistry		
Staff Category	Research	**Reference No**	845552
Reports To	Professor Tell Tuttle, Programme Lead	**Grade**	RS07
Salary Range	£39,906 - £46,049	**Contract Type**	Fixed term (12 Months)
FTE	1.0 FTE (full time)	**Closing Date**	14/09/2026
Working Arrangements	Full time		
Work Location	University of Strathclyde, Glasgow		

Job Advert

The Department of Pure and Applied Chemistry is seeking an exceptional and highly motivated Research Associate to join the ARIA-funded CoreShell Fibre Foundry programme. You will develop high-throughput molecular-simulation analysis workflows and physically meaningful descriptors connecting protein sequence with assembly behaviour and structure. The role will analyse coarse-grained molecular-dynamics trajectories, quantifying features such as curvature, lumen dimensions, packing order, scaffold stability, interfacial organisation and assembly persistence. Working within a fast-paced interdisciplinary team of computational chemists, machine-learning researchers, protein scientists and engineers, you will convert simulation outputs into reliable descriptor datasets and practical design rules for experimental validation. You will have a PhD in a relevant computational discipline, strong Python skills, experience developing quantitative descriptors from molecular or structural data, and experience handling large trajectory datasets. Knowledge of coarse-grained molecular dynamics and experience with Martini, GROMACS, MDAnalysis or related tools would be advantageous. The post is full time and fixed term for 12 months, from 1 October 2026 until 30 September 2027.

Applicants may use tools such as AI to support their application; however, all submissions must accurately reflect their own experience and understanding. The University reserves the right to verify the authenticity of application materials and may reject applications where concerns arise.

Job Description

Brief Outline of Job:

To develop high-throughput analysis workflows and molecular descriptors for coarse-grained simulations undertaken within the CoreShell Fibre Foundry programme. The postholder will extract physically meaningful geometric, topological and structural features from protein-assembly trajectories, build reproducible descriptor datasets for machine-learning models, and work with computational and experimental colleagues to translate simulation outputs into design rules for programmable protein assemblies.

Main Activities/Responsibilities:

1.	Develop high-throughput analysis workflows for coarse-grained molecular-dynamics simulations of candidate protein assemblies.
2.	Extract physically meaningful geometric, topological and structural descriptors from protein-assembly trajectories.
3.	Quantify curvature, lumen dimensions, scaffold and tube stability, packing order, aggregation state, interfacial organisation and assembly persistence.
4.	Develop structure-property relationships linking protein-sequence features to fibre-relevant assembly behaviour.
5.	Generate reliable, well-structured descriptor datasets to support predictive and active-learning model development.
6.	Compare simulated assembly behaviour with experimental microscopy, scattering and other characterisation data.
7.	Develop, test, document and maintain robust, reusable and version-controlled Python analysis pipelines.
8.	Collaborate with molecular-simulation, machine-learning and experimental researchers to support sequence-design decisions and experimental validation.
9.	Contribute to project meetings, milestone reviews, technical reports, research publications, presentations and responsible research-data and software management.

10.	Plan and conduct research independently within agreed programme objectives and undertake other duties appropriate to the grade as required by the Programme Lead.

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	PhD in computational chemistry, molecular simulation, physics, biophysics, materials modelling, computational biology, mathematics or a closely related field.
E2	Evidence of research outputs appropriate to career stage.
D1	Experience with peptide, protein, polymer, colloidal or other self-assembling systems.
D2	Knowledge of coarse-grained molecular dynamics, particularly Martini or a related force field.

Experience

E3	Strong programming experience in Python.
E4	Experience developing quantitative descriptors from molecular, simulation or structural data.
E5	Experience analysing and managing large molecular-simulation trajectory datasets.
D3	Experience with GROMACS, Martini, VMD, MDAnalysis, OVITO or comparable simulation and analysis tools.
D4	Experience using topological, geometric, clustering, graph-based or structural-order analysis for protein, biomolecular or self-assembling systems.

Job Related Skills and Achievements

E6	Ability to design, implement and maintain robust, documented, reusable and reproducible computational workflows.
E7	Strong data-analysis, visualisation and scientific-communication skills, including the ability to explain simulation outputs to non-specialist collaborators.
D5	Experience using high-performance computing resources and managing high-throughput computational workloads.
D6	Experience generating well-structured descriptor datasets for downstream machine-learning models.
E8	Ability to compare simulation-derived measures with experimental microscopy, scattering or other characterisation data.

Personal Attributes

E9	Ability to plan and conduct research independently while working effectively within a collaborative and interdisciplinary team.

E10	Strong attention to detail in computational analysis, software development and scientific data handling.
D7	Enthusiasm for interdisciplinary research involving molecular simulation, machine learning and experiment.
D8	Interest in programmable materials, protein assembly, biomineralisation or continuous manufacturing.

Other Relevant Factors

E11	Commitment to research integrity, reproducible practice, responsible data and software management, and effective contribution to programme reporting and dissemination.

Application Procedure

Applicants should visit Strathclyde's vacancies portal and complete an online application form, including the names of two referees who may be contacted unless the applicant indicates otherwise. Applicants should also submit a CV and a covering letter explaining how their qualifications, research experience, skills and achievements meet the requirements of the role. Applicants should also complete the Equal Opportunities Monitoring Form.

The University of Strathclyde encourages the recruitment of disabled and neurodivergent candidates. If you require any reasonable adjustments or support at any stage of the recruitment or application process, please contact us at humanresources@strath.ac.uk, and we will be happy to assist you. This includes supporting you with the option to submit a paper application or a CV instead of completing the online application form.

Interviews

Formal interviews for this post will be held on 21/09/2026

The University is a Disability Confident Employer and operates a guaranteed interview scheme for disabled candidates who meet all the essential criteria for the post that they are applying for.

Other Information

Further information on the application process and working at Strathclyde can be found on our website (http://www.strath.ac.uk/hr/workforus).

Informal enquiries about the post can be directed to Professor Tell Tuttle, Programme Lead (tell.tuttle@strath.ac.uk).

Conditions of Employment

Conditions of employment relating to the Research staff category can be found at: Conditions of Employment.

Rewards and Benefits

Our comprehensive benefits package, including generous annual leave, family-friendly benefits, flexible work options, and a commitment to continuous learning, reflects our appreciation for the valuable contributions of our colleagues.

We understand that each staff member has unique priorities and lifestyles, so our diverse benefits ensure there is something for everyone, details of which can be found on our Rewards and Benefits webpage.

- **Financial Rewards:** We provide attractive financial packages, including competitive salaries, relocation support for employees and a generous pension scheme, with university contributions of 14.5%.
- **Work-Life Balance:** We are dedicated to enhancing healthy work-life balance for our employees. We offer generous annual leave, an additional annual leave purchase option, flexible and agile work arrangements.
    - Annual Leave: Generous entitlement of 31 days, in addition to 11 public holidays and University closure days.
    - Additional annual leave purchase: Option to request purchase of 2 weeks' additional annual leave per year.
    - Flexible and agile working: The University provides flexible work arrangements. You can request arrangements that fit you and your role, such as hybrid, part-time, compressed hours, term-time, adjusted shifts, staggered hours. These requests can be made from the first day of your employment.
- **Family Friendly Benefits:** We offer a variety of enhanced family-friendly benefits to support our employees in balancing work and family responsibilities. These include Maternity Leave, Paternity/Maternity Support, Adoption Leave, Shared Parental Leave, Parental Leave, Carers Leave and support, Family Friendly Research & Scholarship Leave, and access to our on-campus nursery.
- **Career Development:** Our commitment to personal development is reflected in initiatives such as professional courses, subsidised educational programs, coaching and mentoring, leadership development, secondment opportunities, and access to our library.
- **Health & Wellbeing:** We place high importance on the safety, wellbeing, and health of all our staff and offer discounted Strathclyde Sport membership, an Employee Assistance Programme (EAP), Occupational Health Service, and Cycle to Work scheme.
- **Recognition Awards:** At Strathclyde, we place a strong emphasis on acknowledging and rewarding our staff's commitment and exceptional contributions. This is demonstrated through our Long-Service Awards and our Values-based Strathclyde Medals.

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 Universities' Superannuation Scheme. Further information regarding this scheme is available from Payroll and Pensions.

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+, disabled candidates and candidates from lower socio-economic groups and care-experienced backgrounds.

The University currently holds an Athena Swan **Silver award**, recognising our commitment to support and transform gender equality within higher education and research.

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.

In delivering **our People Strategy**, we will contribute, act, and make decisions guided by these values.

- **People-oriented:** committed to our staff and students, providing opportunities, and investing in their development.
- **Bold:** confident and challenging in what we do, and supportive of embracing appropriate and managed risk in our decision-making.
- **Innovative:** focused on discovering and applying knowledge with impact and encouraging creative thinking and new ideas.
- **Collaborative:** working together, with our colleagues and external partners, with integrity and in an open, respectful way.
- **Ambitious:** for our institution, staff and students as well as supporting the ambitions of our partners.

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/policies/. 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 www.strath.ac.uk/staff/policies/hr.

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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/staff/policies/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/grantholder (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 11 public holidays per year which should be taken on days that the University is closed for this purpose. The University presently closes for 4 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 5 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 5 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:

Period of Continuous Employment at start of absence from work	**Full Pay**	**Half Pay**
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.

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 2026 is £74,208 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). 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 SharePoint (staff login required). Full information regarding USS can be found on the USS website – 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/staff/policies/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/staff/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 2026