

Research Role Profile				
Job Title:	Research Fellow A			
Responsible to:	Head of research group, or principal investigator			
Responsible for:	Not applicable			

#### **Job Summary and Purpose:**

To undertake research in accordance with the specified research project(s) under the supervision of the principal investigator.

# Main Responsibilities/Activities

To undertake a range of research activities within a specified research area, assuming responsibility for specific areas of projects and making use of new research techniques and methods, in consultation with the research award holder or supervisor. This may include fieldwork, interviews, laboratory experimentation, critical evaluation and interpretation, computer-based data analysis and evaluation or library research.

Using initiative and creativity to identify areas for research develop new research methods and extend the research portfolio. Analysing and interpreting results of own research. Write up results and prepare papers for submission to appropriate journals and conferences, and other outputs as required and/or appropriate. Attend appropriate conferences for the purpose of disseminating research results of personal development. The post holder may also contribute to writing bids for research grants and will contribute to collaborative decision making with colleagues in areas of research.

Continually to update knowledge and develop skills, and translate knowledge of advances in the area into research activity.

To plan and manage own research activity in collaboration with others. To carry out administrative tasks associated with specified research funding, for example risk assessment of research activities, organisation of project meetings and documentation. Implementation of procedures required to ensure accurate and timely formal reporting and financial control.

To contribute to teaching in the Faculty by carrying out student supervision and/or demonstrating within the post holder's area of expertise and under the direct guidance of a member of departmental academic staff, as appropriate.

The post holder may occasionally be required to supervise more junior research staff.



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# **Person Specification**

#### The post holder must have:

A doctoral degree in a relevant discipline (although individuals who have almost completed a doctoral degree may be appointed). Consideration may also be given to individuals who do not hold a doctoral degree but have required skills based on a number of years experience in specified / relevant fields

The post holder will have authority over some aspects of project work and must be capable of providing academic judgement, offering original and creative thoughts and be able to interpret and analyse results.

## **Relationships and Contacts**

Direct responsibility to the principal investigator or academic supervisor. The post holder may be asked to serve on a relevant Faculty committee. There may be additional reporting and liaison responsibilities to external funding bodies or sponsors. The post holder may work on original research tasks with colleagues in other institutions.

#### **Special Requirements**

To be available to participate in fieldwork as required by the specified research project

#### All staff are expected to:

- Positively support equality of opportunity and equity of treatment to colleagues and students in accordance with the University of Surrey Equal Opportunities policy.
- Help maintain a safe working environment by:
  - Attending training in Health and Safety requirements as necessary, both on appointment and as changes in duties and techniques demand
  - Following local codes of safe working practices and the University of Surrey Health and Safety Policy
- Undertake such other duties within the scope of the post as may be requested by your Manager.



## Research Role Profile

#### Addendum

This document provides additional information relating to both specific aspects of the post/faculty and any post specific person specification criteria. The information contained within this document should always be read in conjunction with the accompanying generic Role Profile.

Job Title:

Postdoctoral Research Fellow in Mixed Quantum-Classical Dynamics

# **Background Information/Relationships**

The post holder is expected to hold a doctoral degree in Applied Mathematics, Theoretical Chemistry/Physics, or related areas. Previous postdoctoral experience is particularly welcome. The research activity is part of a new international collaboration funded by the Leverhulme Trust and will involve frequent exchanges (both online and in-person) with the project partners Irene Burghardt (Frankfurt), François Gay-Balmaz (Singapore), and Raymond Kapral (Toronto).

The post holder will have authority over some aspects of project work and must be capable of providing academic judgement, offering original and creative thoughts and be able to interpret and analyse results.

He/she will analyse and compare different dynamical models for quantum-classical interaction in both reversible and irreversible regimes. This will involve a combination of mathematical theory, physical insight, and computational techniques. Based on the theory of Hamiltonian/Lagrangian models of complex fluids, quantum-classical hydrodynamic systems will be studied in various cases of physical and chemical relevance by both analytical and numerical tools. The post holder will analyse the implications of several unique features occurring in quantum-classical solvation models, with particular emphasis on solute-solvent interaction. This investigation includes correlations and decoherence effects.

The post holder will report to the theme leader and liaise with other members of the same and different themes of the project.

#### Person Specification

This section describes the sum total of knowledge, experience & competence required by the post holder that is necessary for standard acceptable performance in carrying out this role. This is in addition to the criteria contained within the accompanying generic Role Profile.

	Essential/ Desirable
A PhD in Applied Mathematics, Theoretical Physics/Chemistry, or related areas	Essential
Solid background in both classical and quantum mechanics, including their mathematical settings.	Essential
Familiarity with the mathematical setting of fluid dynamics and complex fluid flows	Desirable
Basic notions in differential geometry and transformations groups.	
Experience with both analytical calculations and numerical simulations in a relevant area	Essential
Publication record in a relevant area	
Cross-disciplinary scientific interests, ranging from foundational problems in quantum mechanics to their implications in applied aspects within different contexts.	



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Willingness to interact and collaborate with other project members from different fields.	Essential
Excellent oral and written communication skills	

# **Key Responsibilities**

This document is not designed to be a list of all tasks undertaken but an outline record of any faculty/post specific responsibilities (5 to 8 maximum). This should be read in conjunction with those contained within the accompanying generic Role Profile.

- Develop new mathematical methods in coupled quantum-classical hydrodynamics.
- Apply the new methods to problems of nonadiabatic solvation dynamics.
- Take part in regular meetings (face-to-face or online) with collaborators on the grant.
- Interact with other members of the team and the wider community in computational chemistry.
- Prepare and publish manuscripts for peer-reviewed journals.
- Present results at project organised workshops, and national and international conferences.

N.B. The above list is not exhaustive.