# Position Details

## CSIRO Early Research Career (CERC) Postdoctoral Fellowship– CSOF4

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| The following information is for applicants | |
| Advertised Job Title | CSIRO Postdoctoral Fellowship in Machine Learning for Quantum Chemistry |
| Job Reference | 95420 |
| Tenure | Specified Term of 3 years  Full-time |
| Salary Range | AU$92,624 to AU$101,459 pa (pro-rata for part-time)  plus up to 15.4% superannuation |
| Location(s) | Clayton, Victoria |
| Relocation Assistance | Will be provided to the successful candidate if required |
| Applications are open to | All Candidates |
| Position reports to the | Project Leader |
| Client Focus – Internal | 80% |
| Client Focus – External | 20% |
| Number of Direct Reports | 0 |
| Enquire about this job | Contact Dr James via email at [james.quach@csiro.au](mailto:james.quach@csiro.au) or phone +61 3 9545 2025 |
| How to apply | Apply online at <https://jobs.csiro.au/>  Internal applicants please apply via **Jobs Central**  If you experience difficulties when applying, please email [careers.online@csiro.au](mailto:careers.online@csiro.au) or call 1300 984 220. |

**Acknowledgement of Country**

CSIRO acknowledges the Traditional Owners of the land, sea and waters, of the areas that we live and work on across Australia. We acknowledge their continuing connection to their culture and pay our respects to their Elders past and present. View our [vision towards reconciliation](https://www.csiro.au/en/about/Indigenous-engagement/Reconciliation-Action-Plan).

**Child Safety**

CSIRO is committed to the safety and wellbeing of all children and young people involved in our activities and programs. View our [Child Safe Policy](https://www.csiro.au/en/about/policies/child-safe-policy).

### Role Overview

**CSIRO Early Research Career (CERC) Fellowships** provide opportunities to scientists and engineers who have completed their doctorate and have less than three years relevant research experience. These Fellowships aim to develop the next generation of future leaders of the innovation system through:

* A differentiated career development program to deliver capability excellence and breadth across all facets of the national innovation system;
* Research training via strategic research and development projects with a clear focus that will deliver real impact through science and engineering excellence;
* An innovative culture supporting the development and demonstration of original thinking and expertise leading to peer-recognition; and
* Opportunities to develop skills and experience in collaborative research teams to effectively work within national and global multi/transdisciplinary and multi-stakeholder environments.

CERC Fellows **are appointed for three years or part time equivalent.**

The CERC Fellow will contribute to developing software for molecular design using machine learning.

Given a molecular geometry, the calculation of microscopic parameters would typically proceed via quantum chemistry calculations which are typically too slow and problematic. Here we bypass this limitation by pre-training an artificial neural network to predict relevant microscopic molecular parameters based only on the structural and alchemical information of candidate molecules. We train and test the neural network on a hybrid data set of known compounds, making use of in-house quantum chemistry calculations and existing, open-access organic molecule databases.

Original research in related topics will also be supported.

### Duties and Key Result Areas

Under the direction of senior research scientists and engineers, this CERC Fellow will:

* + Carry out innovative, impactful research of strategic importance to CSIRO that will, where possible, lead to novel and important scientific outcomes.
  + Recognise and exploit opportunities for innovation and the generation of new theoretical perspectives, and progress opportunities for the further development or creation of new lines of research.
  + Utilise design thinking methodology to plan and prepare research proposals, and apply non-academic impact methodology to research projects.
  + Carry out research investigations requiring originality, creativity and innovation.
  + Record, manage, and analyse data/information using relevant domain data science techniques.
  + Proactively undertake development to grow effective researcher capabilities to support career goals.
  + Adhere to the spirit and practice of CSIRO’s Values, Code of Conduct, Health, Safety and Environment procedures and policy and diversity initiatives.
* Other duties as directed.

The CERC Fellow learning, development and training programis developed between the CERC Fellow and their CSIRO supervisor. The program will focus on enhancing the Fellow’s capabilities to the level expected of an independent researcher and will include on-the-job and course-based development encompassing:

* Discipline-specific techniques and protocols
* Professional growth
* Project management
* Communication and influencing skills
* Working and collaborating with others

## **Selection Criteria**

#### Essential

*Under CSIRO policy only those who meet all essential criteria can be appointed.*

1. A doctorate (or will shortly satisfy the requirements of a PhD). The doctorate must be in computational physics, computational chemistry and/or computer science.

Please note: To be eligible for this role you must have **no more than 3 years** (or part time equivalent) of relevant research experience.

1. A background in machine learning and artificial intelligence.
2. Operational knowledge of Python programming language required with good knowledge of either PyTorch and/or TensorFlow frameworks.
3. Tangential knowledge of quantum chemistry, computational chemistry and/or molecular physics.
4. High level written and oral communication skills with the ability to represent the research team effectively internally and externally, including the presentation of research outcomes at national and international conferences.
5. A sound history of publication in peer reviewed journals and/or authorship of scientific papers, reports, grant applications or patents.
6. A record of science innovation and creativity, including the ability & willingness to incorporate novel ideas and approaches into scientific investigations.

## **Desirable**

1. Portfolio of previous machine learning project(s).
2. Familiarity with lower-level languages (C/C++), Unix operating systems and comfortable with bash terminal.
3. Knowledge/use of existing quantum chemistry packages (e.g. Orca, Gaussian, MolPro).

## **Required Competencies**

* **Teamwork and Collaboration:** Cooperates with others to achieve organisational objectives and may share team resources in order to do this. Collaborates with other teams as well as industry colleagues.
* **Influence and Communication:** Uses knowledge of other party's priorities and adapts presentations or discussions to appeal to the interests and level of the audience. Anticipates and prepares for others reactions.
* **Resource Management/Leadership:** Allocates activities, directs tasks and manages resources to meet objectives. Provides coaching and on the job training, recognises and supports staff achievements and fosters open communication in the team.
* **Judgement and Problem Solving:** Investigates underlying issues of complex and ill-defined problems and develops appropriate response by adapting/creating and testing alternative solutions.
* **Independence:** Recognise and makes immediate changes to improve performance (faster, better, lower cost, more efficiently, better quality, improved client satisfaction).
* **Adaptability:**Copes with ambiguity or situations that lack clarity. Adapts readily to changing circumstances and new responsibilities (which may include activities outside own preferences) in the interests of achieving team objectives. Recognises the need for and undertakes personal development as a result of changes.

To be appointed as a CERC Fellow within CSIRO, candidates are required to have **submitted** their doctoral thesis at the time of commencement, as a minimum requirement, if PhD conferment has not been obtained. If a candidate has submitted, but their PhD has not yet been formally attained, the starting salary will be CSOF4-1 ($89,680). Upon CSIRO receiving written confirmation that the PhD has been awarded (within a six month period from commencement date), the salary will be increased to the negotiated level and the difference will be back-paid to the Officer’s start date.

Special Requirements

Appointment to this role is subject to provision of a pre-employment background check and may be subject to other security/medical/character clearance requirements.

* The successful candidate will undertake a pre-employment background check. Please note that individuals with criminal records are not automatically deemed ineligible. Each application will be considered on its merits.
* If the successful candidate is not an Australian Citizen or Permanent Resident, they may be required to undergo additional security clearances, which may include medical examinations and an international standardised test of English language proficiency (i.e. IELTS test).- https://ielts.com.au/

**Our value proposition**

We want CERC Fellows to join our world class science, engineering and digital teams to solve big, complex problems that make a real difference to the future of Australia and the world.

You'll get to work with some of the most talented minds in their fields, not just in Australia, but in the world. At CSIRO, we spark off each other, learn from each other, trust each other and collaborate closely to achieve more than we could individually.

Find out more about our CSIRO Early Research Career (CERC) Fellow Experience Employee Value Proposition (EVP) [here](https://www.csiro.au/postdoctoral-fellowships).

## **About CSIRO**

We solve the greatest challenges through innovative science and technology. Visit [CSIRO Online](http://www.csiro.au/) for more information.

CSIRO is a values-based organisation.  In your application and at interview you will need to demonstrate behaviours aligned to our values of:

* People First
* Further Together
* Making it Real
* Trusted