# Position Details

## Research Projects- CSOF4

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| The following information is for applicants | |
| Advertised Job Title | Experimental Scientist – Modelling and Simulations |
| Job Reference | 67331 |
| Tenure | Specified Term of 18 months  Full-time |
| Salary Range | AU$83,687 to AU$94,679 pa (pro-rata for part-time) + up to 15.4% superannuation |
| Location(s) | Docklands, VIC |
| Applications are open to | * Australian/NZ Citizens and permanent residents * Australian temporary residents who have full work-rights for the duration of this contract and do not require visa sponsorship. |
| Position reports to the | Team Leader, Modelling and Simulations |
| Client Focus – Internal | 90% |
| Client Focus – External | 10% |
| Number of Direct Reports | 0 |
| Enquire about this job | Dr Michael Kuiper via email at [michael.kuiper@csiro.au](mailto:michael.kuiper@csiro.au) |
| 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. |

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### Role Overview

This role in Materials Modelling and Informatics will assist in the development of a new industry-specific materials informatics platform for screening and designing metal oxide materials for a next generation solar redox reactor. In this role, you will draw on large data bases of computational results and undertake large numbers of simulations using density functional theory, to create a comprehensive resource for multivariate analytics and machine learning.

The Experimental Scientist will integrate established physico-chemical modelling methods with these data analysis methods to link process conditions to verifiable performance criteria and collaborate with experimentalists to verify your results.

### Duties and Key Result Areas:

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

* Engagewith experimental partners and international collaborators to create a database of existing results suitable for screening and processing using established thermochemical methods.
* Simulate the properties of a range of perovskite materials using density functional theory.
* Predictthe structure/property relationships of perovskite materials using the most appropriate and reliable suite of machine learning methods.
* Contribute tothe development of a bespoke materials informatics platform that can be repurposed in the future as other opportunities arise.
* Undertake regular reviews of relevant literature and patents.
* Produce high quality scientific and/or engineering papers suitable for publication in quality journals, for client reports and granting of patents.
* Prepare appropriate conference papers and present those at conferences as agreed with your supervisor.
* Contribute to the development of innovative concepts and ideas for further research.
* Make a contribution to the effective functioning of the research team and help deliver CSIRO’s organisational objectives and plans.
* Work collaboratively with colleagues within your team, the business unit and across CSIRO.
* Communicate effectively and respectfully with all staff, clients and suppliers in the interests of good business practice, collaboration and enhancement of CSIRO’s reputation.
* Adhere to the spirit and practice of CSIRO’s Values, Health, Safety and Environment plans and policies, Diversity initiatives and Zero Harm goals.
* Undertake an appropriate training and development program developed by CSIRO.
* Other duties as directed

## **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.

## **Selection Criteria**

#### Essential

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

1. A doctorate in a relevant discipline area, such as computational chemistry, computational physics or materials data science.
2. A detailed knowledge and extensive experience in the simulation of materials using density functional theory (DFT).
3. Demonstrated proficiency using high performance computing environments.
4. Proven experience, as evidenced by examples, in machine learning and data science methods and their application to large data sets.
5. Demonstrated experience (beyond university courses) in writing and maintaining user-friendly code using python, R or C++.
6. **The ability to work effectively as part of a multi-disciplinary, regionally dispersed research team, plus the motivation and discipline to carry out autonomous research.**
7. A record of science innovation and creativity, plus the ability & willingness to incorporate novel ideas and approaches into scientific investigations.

## **Desirable:**

1. Detailed knowledge of thermochemical water splitting reactions.
2. Demonstrated experience in optimisation algorithms including genetic algorithms (GA) and Bayesian optimisation.

Special Requirements

Appointment to this role may be subject to conditions including provision of a national police check as well as other security/medical/character clearance requirements.

* The successful candidate will be asked to obtain and provide evidence of a National Police Check or equivalent. Please note that people 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/

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