



## POSITION DESCRIPTION

<b>Position Title:</b>	Scientific Computing Scientist
<b>Cluster / Business Unit / Division</b>	Nuclear Science and Technology Australian Centre for Neutron Scattering / Neutron Scattering
<b>Section or Unit:</b>	Science / Diffraction Group
<b>Classification:</b>	Band 7
<b>Job Family:</b>	Science
<b>Position Description Number:</b>	PD-0936
<b>Work Contract Type:</b>	Professional
<b>STEMM/NON-STEMM:</b>	STEMM
<b>STEMM Category:</b>	Research & Sciences

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### POSITION PURPOSE

The primary objective of Scientific Computing Scientist is to assist with the exploitation of neutron scattering instruments by complementing experimental data with atomistic simulations, help develop the user-community and provide research and development leading to significant outcomes that meet with ANSTO's strategic direction. This is a crucial support-role that also requires the incumbent to assist the scientific community in the installation and basic use of other general scientific software that requires the high-performance computing facilities.

### ORGANISATIONAL ENVIRONMENT

ANSTO leverages great science to deliver big outcomes. We partner with scientists and engineers and apply new technologies to provide real-world benefits. Our work improves human health, saves lives, builds our industries and protects the environment. ANSTO is the home of Australia's most significant landmark and national infrastructure for research. Thousands of scientists from industry and academia benefit from gaining access to state-of-the-art instruments every year.

Nuclear Science & Technology (NST) incorporates ANSTO's research, innovation, landmark research infrastructure and associated platforms and capabilities. NST conducts research and development in relation to nuclear science and technology and connects people, transfers knowledge and provides nuclear-based products and services for the benefit of Australia. The Research Infrastructure portfolio consists of platforms established on scientific infrastructure and capabilities, delivering excellence in outcomes through excellence in user experience. This includes a range of scientific assets, infrastructure, capability development & delivery for multi-decadal, multi-disciplinary, multi-user platforms for a collaborative user community and for internal research and development endeavours.

Australian Centre for Neutron Scattering (ACNS) operates neutron and X-ray scattering instruments with specialised sample environment equipment utilising ANSTO's modern high flux reactor and reliable cold neutron source. ACNS conducts structure and function investigations for industry, health, environment, biotechnology, nanotechnology, energy, advanced materials, engineering, food and heritage / archaeology sectors. ACNS is within the top 3 neutron facilities in the world and unique within the Southern Hemisphere with an internationally competitive instrument suite. Extensive user program of >500 users (1500 visits) per year from Australian universities and institutes, international institutions and internal ANSTO researchers. ACNS also services industry needs in engineering, infrastructure, food, automotive and other sectors.

## ACCOUNTABILITIES & RESPONSIBILITIES

### Key Accountabilities

- Provide scientific and technical support to ACNS scientists and users with atomistic modelling such as DFT calculations, force-field and ab initio molecular dynamics, lattice dynamics calculations, to complement ACNS research and user program.
- Use specialised knowledge and expertise to provide detailed advice to users and make scientific and technical decisions for users to ensure they gain the most out of the neutron scattering instruments for their research.
- Conduct leading edge research and improve scientific visibility to increase the profile of ANSTO & ACNS.
- Contribute to raising ACNS and ANSTO visibility internationally by presenting at conferences.
- Maintain knowledge of industry best practice and technological developments in the scientific computing to ensure research benefits ANSTO and in particular the area of atomistic modelling in the context of neutron scattering research.
- Use research networks to coordinate and collaborate with local, national and international scientists to produce research outcomes and increase usage of ACNS.
- Produce collaborative research of emerging international standard, publication in refereed journals and other reputable publications, and participation in professional fora, steering committees and other professional associations.
- Contribute to the research culture within ACNS by coaching and knowledge sharing with staff and work collaboratively to share technical expertise.
- Work with ANSTO's scientific community to better utilise available High Performance Computing resources through either education or active involvement in the development process of 'home grown' or specialist software solutions for such environments.
- Coordinate and undertake outreach activities to promote and educate ACNS scientists and the user community of atomistic modelling.
- Install and maintain atomistic modelling codes on the ANSTO cluster and ensure that , commercial licenses are renewed.

### Decision Making

Scientific Computing Scientist makes informed recommendations on improvements to High Performance Computing environment in order to provide effective High Performance Computing facilities for use by the scientific community.

### Key Challenges

- Working in a heavily regulated environment and adherence to all regulations is mandatory.
- Working in accordance with operational requirements and tight deadlines.
- Maintaining knowledge and expertise with new systems that become available.
- Educating the ACNS staff and neutron user community on how best to leverage ANSTO's High Performance Computing Infrastructures.

## KEY RELATIONSHIPS

Who	Purpose
<b>Internal</b>	
Manager, ACNS Instrument Group	<ul style="list-style-type: none"><li>• Receive guidance and direction</li><li>• Provide expert, authoritative and evidence based advice</li><li>• Recommend and gain endorsement for plans and goals and other initiatives.</li></ul>

ACNS scientists	<ul style="list-style-type: none"> <li>• Provide expert advice and analysis on a full range of matters</li> <li>• Contribute to group decision making processes, planning and goals</li> <li>• Collaborate and share accountability</li> <li>• Negotiate and resolve conflicts</li> </ul>
ANSTO IT	<ul style="list-style-type: none"> <li>• Coordinate scientific computing activities, e.g., codes installation, license server operation, computing jobs queuing, etc.</li> </ul>
<b>External</b>	
ACNS neutron users	<ul style="list-style-type: none"> <li>• Provide guidance and support</li> </ul>

## POSITION DIMENSIONS

<b>Staff Data</b>	
Reporting Line	Reports to the Diffraction Group Manager
Direct Reports	Nil
Indirect Reports	Nil

<b>Financial Data (2023/2024)</b>	
Revenue / Grants	N/A
Operating Budget	N/A
Staffing Budget	N/A
Capital Budget	N/A
Assets	N/A

<b>Special / Physical Requirements</b>	
Location:	Lucas Heights Working in different areas of designated site/campus as needed
Travel:	Travel both internationally and nationally
Physical:	Office based physical requirements (sitting, standing, minimal manual handling, movement around office and site, extended hours working at computer) Public speaking
Radiation areas:	May be required to work in radiation areas under tightly regulated conditions
Hours:	Nil special requirements
Clearance requirements:	Satisfy ANSTO Security and Medical clearance requirements

<b>Workplace Health &amp; Safety</b>	
Specific role/s as specified in <a href="#">AP- All Workers 2362</a> of the ANSTO WHS Management System	Other specialised roles identified within the guideline a position holder may be allocated to in the course of their duties

## ORGANISATIONAL CHART

Refer to published Organisational Chart.

## KNOWLEDGE, SKILLS AND EXPERIENCE

1. PhD in Chemistry, Physics, Materials Science, Biology or a related discipline.
2. Postdoctoral experience in a relevant discipline
3. Experience in conducting research focused on atomistic modelling utilising DFT codes.

4. Experience in conducting or supporting atomistic modelling research on High Performance Computing clusters, e.g. codes compilation, installation, troubleshooting, maintaining license servers, familiarity with queueing systems, e.g. PBS.
5. A track record of publication and an ability to contribute to research profiles.
6. Experience of neutron scattering (desirable)
7. Excellent interpersonal and communication skills.
8. Demonstrated experience in managing effective relationships with key stakeholders

#### VERIFICATION

This section verifies that the line manager and appropriate senior manager/executive confirm that this is a true and accurate reflection of the position.

Line Manager		Delegated Authority	
Name:	James Hester	Name:	Jamie Schulz
Title:	Manager, ACNS Instrument Group - Diffraction	Title:	Leader, Neutron Scattering
Signature:		Signature:	
Date:	1/11/2023	Date:	1/11/2023

#### Appendix 1

ANSTO Job Families
Accounting & Finance
Administration
Communications & Marketing
Compliance & Regulation
Engineering and Technical
Human Resources
ICT & Digital Solutions
Information & Knowledge Management
Legal
Manufacturing
Monitoring & Audit
Operations
Organisational Leadership
Project & Program
Research
Science
Security & Intelligence
Senior Executive
Service Delivery
Strategic Policy
Trades & Labour