Submission
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Capability Issues Paper

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Executive Summary

In the coming decade, theory and modelling will harness massive advances in high performance computing to enable an unprecedented acceleration in discovery and development of new materials for the energy, environment, health and IT sectors. Effectively, high performance computation – in concert with new characterization and fabrication techniques - are the game changers in materials science at this point in time. The increasingly pivotal role of materials simulations in the design of functional materials is now firmly recognized, as evidenced by the significant infrastructure funding and research effort associated with the Materials Genome initiative[1] in the US as well as analogous research thrusts in Europe and China (e.g.,[2,3]).

Importantly, high performance computational modelling must work hand-in-glove with materials synthesis, fabrication and characterization in order to truly accelerate the materials design and discovery cycle: each unlocking greater potential within the others. This mode of synergistic operation has been established with great success in the five Department of Energy funded nanoscience centres in the United States (one each at Lawrence Berkeley National Laboratory; Argonne National Laboratory; Oak Ridge National Laboratory; Brookhaven National Laboratory and the joint centre at Sandia National Laboratory-Los Alamos National Laboratory). Amongst the five DOE centres, the Centre for Nanophase Materials Science at ORNL has fostered the largest and most productive theory and computing group.

The current National Research Infrastructure Roadmap consultation process provides an opportunity for a careful evaluation of capabilities available to users from academia and industry here in Australia:

- NCRIS has invested to ensure the necessary infrastructure - as well as the technical expertise needed to facilitate user projects - is available for state of the art materials nanofabrication (ANNF) and characterization (AMMRF and NIF).
- Through the NCI, NCRIS also provides essential hardware capabilities for high performance simulations.

However, there exists currently no mechanism within NCRIS by which users in need of significant computational (in-silico) characterization support for materials projects can obtain such results. Yet, data and associated interpretation from materials simulations is today a prerequisite for any significant research to be published in upper-tier science journals. This represents a critical shortfall in the provision of capabilities. In the present environment, experimental groups obtaining computational characterization data and the associated insights relies largely on happenstance: whether they happen to know another academic group which can do such simulations and whether said group has bandwidth (both in terms of personnel and access to HPC resources) to take on the project.

By analogy, one notes that it would be unthinkable to acquire a multimillion dollar electron microscope and not have one or more highly skilled scientists with domain expertise to act as an interface between the machine and groups that need to use it to examine their materials samples - but do not have the technical knowledge and experience to get the best out of the machine. Through the NCI and Pawsey centres, Australia has invested many tens of millions of dollars in high performance computing hardware; but the NCRIS system lacks highly qualified scientists with domain area expertise who are supported to interface with non-expert groups needing sophisticated in-silico characterization data to support their materials projects. True, the NCI does have some excellent support staff with very strong skill bases – but their main mandate is to make sure that codes are compiled and running efficiently and they interface only with users who already have the skills and experience to run high performance simulations. The current cadre of NCI support staff have no bandwidth to deal with the capability gap that is identified herein.

High performance computational materials modelling will be a transformative enabling capacity over the coming decade, impacting profoundly on the power, potential and direction of nanoscale materials synthesis, fabrication and functionality. It will aid, interpret and predict. However, this power cannot be unlocked only by having computational resources (i.e., hardware capabilities) available: personnel with a high level of materials simulation expertise (quantum chemistry, condensed matter physics, classical molecular dynamics as well as continuum and device-scale methods) need to be integrated into a user program capability – as has been done within the US DOE centres – in order to allow Australia to remain competitive with world best provision of user project capabilities for the advancement of science and engineering. Through harnessing the exponential acceleration of materials simulation capabilities to benefit a large number of projects from the user community, NCRIS has the opportunity in the coming decade to significantly amplify the benefits of its investments in characterization and imaging (ANFF; AMMRF; NIF) on the one hand and high performance computing (NCI, Pawsey) on the other.

What form such an "in-silico characterization" capability could or should take in the Australian context is not yet clear. A few brief indications are relevant here:

- There is no intrinsic need for it to be physically concentrated in one place – activity might be spread over perhaps two or three nodes nationally with complementary expertise and critical mass.
- The capability must work seamlessly with the NCI and Pawsey to ensure that the necessary computing facilities are available, well utilized and that the very broad (presently largely untapped) user base is well served.
- Proximity to the major ANFF and AMMRF nodes and other major federally or state funded user facilities could be beneficial, particularly in light of the need to jointly support user projects requiring a matrix of synthesis, fabrication, characterization and modelling.

This is in fact an opportunity for a creative Australian solution that may even work better than international models.

As a contextual footnote, at UNSW, this need has been recognized with the constitution of the Integrated Materials Design Centre (IMDC)[4]. The IMDC drives high performance computational materials modelling in an integrated discovery and design process, working hand-in-glove with major areas of strength in materials synthesis, characterization and testing at UNSW and more broadly with academia and industry. It interfaces efficiently with the NCI and the Pawsey Centre. While the IMDC's core focus is high performance materials modelling, its core philosophy is to pursue a holistic approach to the materials design cycle involving a tight collaborative exchange between the key parts of the materials discovery process: synthesis; characterization; testing and modelling.

1. Further information on the US Materials Genome Initiative may be found at http://www.whitehouse.gov/mgi

2. Further information on the Swiss Materials Genome initiative may be found at http://actu.epfl.ch/news/epfl-has-become-the-swiss-capital-for-research-on-/
3. Further information on the Chinese Materials Genome initiative may be found at http://engineering.org.cn/EN/abstract/abstract12169.shtml
4. Further information on the IMDC may be found at http://www.imdc.unsw.edu.au

Responses to Questions

General questions

Question 1:	Are there other capability areas that should be considered?

- NCRIS has invested to ensure the necessary infrastructure - as well as the technical expertise needed to facilitate user projects - is available for state of the art materials nanofabrication (ANNF) and characterization (AMMRF and NIF).
- Through the NCI, NCRIS also provides essential hardware capabilities for high performance simulations.

However, there exists currently no mechanism within NCRIS by which users in need of significant computational (in-silico) characterization support for materials projects can obtain such results. Yet,

- Data and associated interpretative insights from materials simulations is today a prerequisite for any significant materials research to be published in upper-tier science journals.
- The case has been made extensively and with great impact internationally (refs 1-3 above) that computational materials and chemistry capabilities are vital for both the acceleration and the translational impact of new materials discoveries.

This represents a critical shortfall in the provision of capabilities. In the present environment, experimental groups obtaining computational characterization data and the associated insights relies largely on happenstance: whether they happen to know another academic group which can do such simulations and whether said group has bandwidth (both in terms of personnel and access to HPC resources) to take on the project.

Question 2:	Are these governance characteristics appropriate and are there other factors that should be considered for optimal governance for national research infrastructure.

- It would be beneficial to establish clear and transparent policies for managing IP arising from the activities of user facilities – whether solely within the facility or in collaboration with user projects.
- The in-silico materials characterization capability flagged above clearly reaches across the domains of several existing NCRIS projects (NCI, ANFF, AMMRF) and hence offers the opportunity to develop significant productive collaborations between these projects that will powerfully leverage the capabilities of each to achieve better user service and better user outcomes. This may imply some tweaking of – or augmentation of - governance structures to ensure efficient operations.

Question 3:	Should national research infrastructure investment assist with access to international facilities?

It would be worthwhile to explore models for international collaboration between cognate user facilities. The US DOE nanoscience user facilities may well be receptive to this. Such a model could be delivered quite quickly in the context of an in-silico materials characterization capability as flagged above, since this is not dependent on physical co-location of staff with hardware; the capability lends itself to engagements at a distance; and the US facilities (almost uniquely worldwide) have established capabilities in this area. Something needs to be contributed from both sides, however, and as noted above Australia presently has no such capability funded through NCRIS. If a decision to build the in-silico materials characterization capability through NCRIS funded projects within Australia is pursued, then this potential for international collaborations would offer opportunities for significant added leverage to enhance the outcomes.

Question 4:	What are the conditions or scenarios where access to international facilities should be prioritised over developing national facilities?

If a capability can feasibly be built and cost effectively managed in Australia, it is always beneficial to do so, since this raises the awareness, the skill base and the overall levels of cooperation and collaboration within the Australian R&D communities. Where a national capability can be leveraged to advantage by international collaborations, this is ideal. Capabilities that hinge on very large scale infrastructure that is beyond the capacity of an economy of Australia's size to develop – or is simply not cost effective to develop nationally - must necessarily be developed "off the back of" internationally available infrastructure through co-investment models.

Question 12:	Are there international or global models that represent best practice for national research infrastructure that could be considered?

The US Department of Energy user facilities – encompassing light sources, neutron sources and nanoscience facilities – represent a notable benchmark in best practice. However, those facilities are very different in overall funding and organizational framework from the university-based Australian NCRIS facilities – based as they are primarily within national laboratories. Those organizational contrasts are not always conducive to better efficiencies and outcomes. As noted above, Australia has the opportunity through the current National Research Infrastructure Roadmap initiative to develop creative solutions that work better than existing international models.

Advanced Physics, Chemistry, Mathematics and Materials

Question 21:	Are the identified emerging directions and research infrastructure capabilities for Advanced Physics, Chemistry, Mathematics and Materials right? Are there any missing or additional needed?

High performance computational materials modelling will be a transformative enabling capacity over the coming decade, impacting profoundly on the power, potential and direction of nanoscale materials synthesis, fabrication and functionality. It will aid, interpret and predict. However, this power cannot be unlocked only by having computational resources (i.e., hardware capabilities) available: **personnel with a high level of materials simulation expertise (quantum chemistry, condensed matter physics, classical molecular dynamics as well as continuum and device-scale methods) need to be integrated into a user program capability – as has been done within the US DOE nanoscience centres – in order to allow Australia to remain competitive with world best provision of user project capabilities for the advancement of science and engineering**. Through harnessing the exponential acceleration of materials simulation capabilities to benefit a large number of projects from the user community, NCRIS has the opportunity in the coming decade to significantly amplify the benefits of its investments in characterization and imaging (ANFF; AMMRF; NIF) on the one hand and high performance computing (NCI, Pawsey) on the other.

Underpinning Research Infrastructure

Question 30:	Are the identified emerging directions and research infrastructure capabilities for Underpinning Research Infrastructure right? Are there any missing or additional needed?

The in-silico materials characterization capability flagged above clearly reaches across the domains of several existing NCRIS projects (NCI, ANFF, AMMRF) and hence offers the opportunity to develop significant productive collaborations between these projects that will powerfully leverage the capabilities of each to achieve better user service and better user outcomes. The challenge to make domain expertise in high performance atomistic materials and chemistry simulations available to the Australian materials R&D community (both academia and industry) is justified by the enormous and growing significance of high performance modelling in the acceleration of new materials design and discovery as well as the translation of new discoveries into workable technologies, with associated impact for industry and the economy. This is a key missing ingredient in Australia's underpinning research infrastructure that will both bridge and leverage upon NCI, ANFF and AMMRF capabilities to produce highly significant R&D outcomes across the very broad domains of materials science, sustainable energy technologies, nano and nano-biotechnologies, electronics, nanomedicine, pharmaceutics and beyond.

Data for Research and Discoverability

Question 33	Are the identified emerging directions and research infrastructure capabilities for Data for Research and Discoverability right? Are there any missing or additional needed?

The in-silico materials characterization capability flagged above clearly has significant requirements in the context of data access, mining and curation. This relates to the rapidly developing field of materials informatics, which has been driven internationally through the Materials Genome Initiative. Hence, developing an efficient nexus between an in-silico materials characterization capability and the data management capabilities of the e-Research Framework will be an important component of the initiative.