



Curtin University



# Faculty of Science and Engineering

2020 Australian Government Research Training Program Scholarships

## Strategic Project Profile

**PROJECT TITLE:** Predictive simulation of crystallisation

**FIELD OF RESEARCH CODE:** 0306

### PROJECT SYNOPSIS:

This proposal seeks to address the lack of a quantitatively accurate theory to describe how solid materials are formed from ions and molecules that are dissolved in a liquid. It is expected that innovative computer models will be generated that are capable of simulating macroscopic observations from results obtained for microscopic reactions alone. The anticipated outcomes would include new methods for predicting the structure and properties of materials, such as minerals or molecular crystals, based on how they were formed in an experiment, as well as how fast this would occur. This should lead to significant benefits by allowing industry to optimise, in silico, the production of materials and reduce undesirable by-products.

### FEASIBILITY AND RESOURCING – DESCRIPTION OF THE SUPPORT THIS PROJECT WILL RECEIVE:

The scholarships would be associated with the ARC Laureate Fellowship of the applicant and the Future Fellowship of Dr Raffaella Demichelis. Therefore a total of almost \$3 million is available in resources to support this activity.

NB: We are not requesting extra scholarships through this process (since several are already earmarked for these grants), but that the availability of scholarships be promoted as part of this scheme in order to attract the best students from within Australia.

#### **WHAT MINIMAL ATTRIBUTES AND SKILLS EXPECTED BY THE CANDIDATE BE COMPETITIVE:**

Candidates would require a strong background in chemistry, physics, materials science or a relevant discipline with previous experience in computational techniques for atomistic simulation being an advantage.

#### **THE SIGNIFICANCE OF THE PROJECT/ PROGRAM FOR THE ENROLLING SCHOOL OR INSTITUTION:**

As noted above, the project is aligned with two ARC Fellowships, as well as supporting research that underpins an ERA 2018 rating of 5 for Physical Chemistry and for Chemical Sciences overall.

**Students are advised to contact the Project Lead listed below prior to submission of their scholarship application to discuss their suitability to be involved in this strategic project.**

#### **PROJECT LEAD CONTACT**

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#### **CO-SUPERVISOR**

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#### **CO-SUPERVISOR**

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