Dr Charlotte Petersen
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PhD Scholarship Opportunity -
Computer simulations to characterise the structure of amorphous materials: Do microscopic vibrations predict macroscopic behaviour?

I am currently recruiting an enthusiastic PhD student in theoretical and computational chemistry/physics in the School of Chemistry at the University of Melbourne, Australia.

Predicting the rigid behaviour of glass from its disordered, amorphous atomic structure is a longstanding unsolved mystery in materials science. We are aiming to define an innovative measure of structure based on how constrained each particle is, which can be quantified by measuring the particles' vibrations. These vibrations should be quantifiable by the "blur" in the material's diffraction pattern. Using this new measure of structure, we plan to link the microscopic structure of glass to its macroscopic properties via computer simulations. Expected outcomes of this project include a new methodology for characterising amorphous materials and an improved understanding of the nature of glass. This should provide significant benefits, such as an increased ability to rationally design amorphous materials with desired properties.

We will use molecular dynamics simulations to model the glassy materials. We will consider both simple models, as well as realistic models of metallic glass. The project will make use of existing software to run the simulations, but a significant amount of programming will be required to analyse the results.

Understanding the nature of glass is a research area that is currently attracting a large amount of interest and funding internationally. This is an exciting opportunity to begin a career in this field at a world class university.

Your Profile
You have an Honours or Masters degree in chemistry, physics or related discipline, with confidence in mathematics, strong analytical skills, and an interest in coding. Previous experience with molecular dynamics simulations or statistical mechanics is desirable.

You are motivated and enthusiastic about working on fundamental research. You have excellent communication skills, and can work independently as well as in a team. English language proficiency is essential.

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Application
Enquiries should be sent to charlotte.petersen@unimelb.edu.au.

Please include:

- Personal statement outlining your motivation for pursuing a PhD in this topic, and addressing your ability to contribute to computational chemistry research. (max 3,000 characters). Provide evidence of your confidence in mathematics, strong analytical skills, and an interest in coding. If applicable, mention any previous experience with molecular dynamics simulations or statistical mechanics.
- Academic transcript
- Reports from 2 academic referees
- CV, including research experience.