PhD Studentship

Dr. Livia Bartok-Partay

**PhD project:** Unlocking accurate macroscopic predictions: expanding the boundaries of developing atomic interaction models

**Supervisors:** Dr. Livia Bartok-Partay

**Funding availability:** UK Students & EU Students

**Deadline:** 31st March 2020

**Project description:**
A PhD studentship is available in the research group of Livia Bartok-Partay, with anticipated start date in October 2020.

Computer simulation on the atomistic level became a powerful tool in modern chemistry in the past decades, and widely used to augment experiments, make initial predictions and modelling matter at difficult conditions. In computer simulations one of the key ingredients to be able to accurately predict the structure and the properties is the quality of the description of atomic interactions: the potential model employed. In order to compromise between computational efficiency, generality and accuracy, empirical or semi-empirical potentials are often used as descriptors in most large-scale and long-time computations. These potentials are commonly determined by fitting a proposed functional form to a group of available data, which may be obtained from either experimental measurements or first-principles calculations. However, it is difficult to predict how these potentials will perform under conditions different from those of the exact fitting conditions. While some of the microscopic properties are likely to be reproduced accurately, the macroscopic behaviour of the potential model can be very different from what is expected, especially the complex phenomena of phase transitions and phase stability, often seriously limiting the use of computational results. Due to the lack of knowledge of the phase diagram of specific models, this is rarely anticipated and can cause grave misinterpretation of the computational findings.
However, with a recently introduced computational method, called nested sampling, the calculation of the phase diagram is no longer a bottleneck, and thus the reliability of the chosen model can be easily established. The studentship will focus on using nested sampling along with a range of computational techniques to determine the reliability of a variety of potential models for metals and alloys, and to take it a huge step further: design a protocol to feed the phase diagram information into the process of improving and designing new potential models.

The student will employ a range of advanced computational modelling methods and state-of-the-art sampling techniques, also contributing to their development. The project will further involve computations on national and international-scale high-performance computing facilities, and enhanced data analysis as well as visualisation.

Requirements:
This project is suitable for students with a background in the physical sciences (chemistry, physics, materials science) and the successful applicants will have a minimum of a 2:1 first degree in a relevant discipline/subject area. The start date is October 2020.

Funding:
The studentship provides funding for 3.5 years to UK and EU students to cover maintenance as well as paying the university fees and providing funding for PhD travel expenses and research support. The tax-free stipend is at the standard research council rates (for 2019/20 that is £15,009 per annum).

How to apply:
For further details please contact Dr. Livia Bartok-Partay: Livia.Bartok-Partay@warwick.ac.uk
Group webpage: https://liviabpartay.wordpress.com/