PhD Studentship
Dr G.C. Sosso and Dr. J.R. Kermode

PhD project: - Machine Learning for Materials Science -

CORSICA: Navigating at will the silicon-carbon phase diagram via machine learning

Supervisor: Dr. G.C. Sosso (Warwick Chemistry) and Dr. J.R. Kermode (Warwick Engineering)

Funding availability: Fully funded (EPSRC-NPIF) for 4 years

Deadline: July 7th 2018.

Project description:

Silicon and carbon are two of the cornerstones of materials science, at the heart of countless technological applications encompassing electronic devices, energy storage, photovoltaics and drug delivery [1]. As such, a monumental body of both experimental and computational work has been devoted to unravel the origins of the functional properties of the many allotropes of Si and C. Strikingly, though, our understanding of the Si-C phase diagram, and even more prominently of Si/C interfaces, is to date quite minimal. This is largely due to the limitations of both electronic structure calculations and classical molecular dynamics in terms of accessible length/time scales and accuracy, respectively. As a result, we cannot acquire the atomistic insight we need to transform a number of potentially game-changing ideas, such as harnessing silicon carbide for quantum computing [2], into industrial applications. This Studentship will contribute to bridge this gap by developing a bespoke machine-learning based interatomic potential [3], hence enabling large-scale, accurate atomistic simulations across the whole of the Si-C phase diagram, including e.g. silicon carbide, binary Si/C liquid mixtures and the disordered Si/C nanostructures. We will build upon the expertise of both Sosso and Kermode in machine learning for materials science [4] and in the modelling of Si/C/SiC [5],
specifically targeting the functional properties of the Si-C system of relevance for novel industrial applications, which will be identified through collaboration with the Fraunhofer Institute for Mechanics of Materials. In a nutshell, the ambitious goal of this Studentship is to develop and validate a set of computational tools to further our understanding of the structure-function relation of a vast library of Si-C materials, thus making a concrete impact in terms of the rational design of e.g. the next generation of brake discs for high-performance cars [6].


Requirements:
Applicants should have an Honours/Master degree (at least II.1 or equivalent) in Materials Science, Physics, Chemistry, Engineering, Mathematics (or other relevant discipline), and should be a UK citizen - or have been a resident in the UK for three or more years.

How to apply:
Please direct informal enquiries and requests for further information to:
Dr. G.C. Sosso (g.sosso@warwick.ac.uk)

Details on the formal application procedure can be found at http://www.go.warwick.ac.uk/pgapply