2016 YCCSA SUMMER SCHOLARSHIP PROJECT SUBMISSION

This form is for prospective project supervisors to submit their projects to be included in the YCCSA Summer Scholarships Programme for 2017.

It is the purpose of the YCCSA Summer School that any projects submitted are novel and interdisciplinary in nature.

Date	*5 Jan 2017*
Supervisors' Names and Departments / Affiliation and Contact Email	*Matt Probert (Dept of Physics, matt.probert@york.ac.uk)* *Steve Smith (Dept of Electronics, stephen.smith@york.ac.uk)*
Project Title	*Bio-inspired global optimization methods and crystal structure prediction*
Project Description	*There has been much interest in recent years in using and developing various bio-inspired algorithms to solve the very challenging problem of global optimization. Inspiration has been drawn from various systems, such as ant colonies, particle swarms, and evolution. Each of these different approaches has been developed into a computational algorithm and tested on either toy models or various domain-specific areas of science and engineering. However, it is hard to know which algorithm is best for which class of problems, as there are very few systematic & fair comparisons of solving the same problem using different algorithms.* *In this project, you will compare and contrast two or more different algorithms, such as Genetic Algorithms (GA), Cartesian Genetic Progamming (CGP), Particle Swarm Optimization (PSO), etc for the same problem – predicting the ground state crystal structure for a collection of interacting atoms. You will implement the different algorithms in a high level scripting language, such as python, and use an existing code (CASTEP) for calculating the atomic interactions. Probert is one of the core CASTEP developers and has expertise in GAs. Smith has expertise in the other evolutionary algorithms such as CGP. In this project you will need to use both to achieve the project aims. Whilst there has been some interest in using GAs for crystal structure prediction, other bio-inspired algorithms have great potential and have never been attempted – hence the novelty and interest of this proposal.*
Required Skills	*You will need to be competent in programming in a high-level scripting language such as python, and have a basic understanding of, and familiarity with, function optimization. Some knowledge of materials (especially the structure of crystals) would be useful but not essential.*
Supervision and Collaboration Arrangements	*The student will be primarily supervised by Probert, but with weekly review meetings with both Probert and Smith. Probert will give guidance on the domain specific application (crystal structure prediction) and using CASTEP and GAs. Smith will give guidance on*

	the other global optimization methods such as CGP, how to translate the concepts into the relevant application domain, and help with designing suitable comparison methods and metrics.
Project Dates	*The summer school runs for 9 weeks, starting on Monday, 10 July 2017 and finishing on Friday, 8 September 2017.*
Other Information	
References	*Initial implementation of Genetic Algorithms in CASTEP see Physical Review B vol 73 art 224104 (2006) (https://doi.org/10.1103/PhysRevB.73.224104)* *Miller JF. Cartesian genetic programming. In Cartesian Genetic Programming 2011 (pp. 17-34). Springer Berlin Heidelberg. (http://www.springer.com/cda/content/document/cda_downloaddocument/9783642173097-c2.pdf)* *General overview of global optimization including bio-inspired algorithms see the textbook "Engineering Optimization: An Introduction with Metaheuristic Applications" by Xin-She Yang (Wiley 2010) ISBN: 978-0-470-58246-6*

When complete, please email the form to sarah.christmas@york.ac.uk