

## **Machine-Learning Acceleration of DFT Calculations in CASTEP**

Abstract: I will discuss our experience to date using on-the-fly fitting and evaluation of a Machine Learning interatomic potential, as a way of significantly accelerating first principles molecular dynamics calculations of materials, without loss of accuracy compared to the underlying first principles method. This is in contrast to the more established approach of carefully fitting an ML potential to a wide body of data calculated using a first principles method, and then using that in a calculation of the dynamics. I will then show how the learned potential can be used in other calculations, at much larger scale.

Bio: Matt Probert is Professor of Computational Condensed Matter Physics at the University of York. He has been one of the core CASTEP Developers Group since 1998, and has made many contributions to the code, especially around MD and structure optimization, and more recently around structure prediction and integrating machine-learning into CASTEP. He is a Visiting Professor at the University of Lille.