

ID: 1.5.1a

Title: Interatomic potentials and quantum mechanical models

Name: Csanyi, Gabor

Affiliation: University of Cambridge

I will discuss our work from the past ten years on interatomic potentials and explicitly quantum mechanical models. The two strands of this work are concurrent multiscale molecular dynamics (with applications to brittle fracture and solvation chemistry), and the construction of a new generation interatomic potential models that aim to faithfully represent ab initio potential energy surfaces. I will focus on what we have learned about the nature of such coupling methods, their limitations and future directions.