Description of project

The study of energy landscapes holds the key to resolving some of the most important contemporary problems in chemical physics, including how a protein folds to its native state, and why structural glasses exhibit a wide range of puzzling behaviour. In particular, using stationary points of the underlying potential energy surface as a computational framework provides efficient methods for locating global minima, analysing global thermodynamics, and characterising the rate constants and pathways for rare events.

For small molecules it is often possible to map out a complete reaction graph containing every permutational isomer and the transition states that link them. For small water clusters, this approach has enabled us to predict and interpret the tunnelling splittings observed in recent far-infra-red vibration-rotation tunnelling spectra recorded by the Saykally group in Berkeley. A basic understanding of fundamental rearrangement mechanisms is also essential to explain the formation and behaviour of molecules ranging from fullerenes to borohydrides and carboranes.

For larger systems we can only obtain partial samples of the complete set of minima and transition states. Nevertheless, it is still possible to construct accurate partition functions and gain insight into relaxation dynamics from these samples. In particular, we have recently identified three different kinds of energy landscape, which give rise to radically different behaviour. Together with previous work, these results explain how some systems can locate their global minimum easily, while others are always trapped as glasses.

A deeper understanding of the relation between thermodynamics, dynamics and the underlying potential energy surface has recently provided new insight into the global optimisation problem. A simple transformation of the potential energy surface has led to the discovery of a number of new global minima for atomic and molecular clusters.

Possible projects include methodology development, programming, and applications, which range from coarse-grained modelling of self-assembly to simulation of biomolecules and soft matter. Please contact dw34@cam.ac.uk to arrange a time if you would like to discuss possible projects for the coming year.

Previous undergraduate projects have produced the following publications:


