

Exploring the Energy Landscapes of Clusters and Unusual Minima

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The potential energy landscape provides a conceptual and computational framework for investigating structure, dynamics and thermodynamics in atomic and molecular science. This talk will summarise new approaches for global optimisation, quantum dynamics, the thermodynamic properties of systems exhibiting broken ergodicity, and rare event dynamics. Applications will be presented that range from prediction and analysis of high-resolution spectra, to coarse-grained models of mesoscopic structures, covering a wide range of structures, including shells, tubes, helices and knots.