Energy Landscapes of Clusters: From Atoms to Amyloid

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Coarse-graining the potential energy surface into the basins of attraction of local minima provides a computational framework for investigating structure, dynamics and thermodynamics in molecular science [1, 2]. Basin-hopping global optimisation employs steps between local minima [3, 4], and predicts novel 'magic number' structures for clusters in the mesoscopic regime, including links and knots [5]. To treat global dynamics we must include transition states of the potential energy surface, which link local minima via steepest-descent paths. We may then apply the discrete path sampling method [6, 7], which provides access to rate constants for rare events. In large systems the paths between minima with unrelated structures may involve hundreds of stationary points of the potential energy surface. New algorithms have been developed for both geometry optimisation and making connections between distant local minima [8, 9], which allow us to treat such systems. Applications will be presented for a variety of atomic and molecular clusters. Recent results for the aggregation of misfolded peptides illustrate how experimental time and length scales can now be addressed for such systems [10, 11].

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