Evolutionary discovery of transition states in water clusters - DTU Orbit (29/08/2017)

**Evolutionary discovery of transition states in water clusters**

As a basic Aristotle element, water is the most abundant and more importantly crucial substance on earth. Without water, there would not be any form of life as we know. Understanding many phenomena in water such as water evaporation and ice melting and formation requires a deep understanding of hydrogen bond breaking and formation. In particular transition states play a key role in the understanding of such hydrogen bond behavior. Transition states, unlike other metastable states, are energy maxima along the minimum energy path connecting two isomers of molecular clusters. Geometry optimization of transition state structures, however, is a difficult task, and becomes even more arduous, especially when dealing with complex biochemical systems using first-principles calculations. In this paper, a novel molecular memetic algorithm (MOL-MA) composing of specially designed molecular-based water evolutionary operators coupled with a transition-state-local search solver and valley adaptive clearing scheme for the discovery of multiple precise transition states structures is proposed. The transition states of water clusters up to four water molecules uncovered using MOL-MA are reported. MOL-MA is shown not only to reproduce previously found transition states in water clusters, but also established newly discovered transition states for sizes 2–4 water molecules. The search performance of MOL-MA is also shown to outperform its compers when pitted against those reported in the literature for finding transition states as well as recent advances in niching algorithms in terms of solution precision, computational effort, and number of transition states uncovered.

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