Characterization of Transition States in Conformational Dynamics using Fuzzy Sets

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Abstract

Recently, a novel approach for the analysis of molecular dynamics on the basis of a transfer operator has been introduced. Therein conformations are considered to be disjoint metastable clusters within position space of a molecule. These clusters are defined by almost invariant characteristic functions that can be computed via Perron Cluster analysis.

We suggest to replace crisp clusters with fuzzy clusters, i.e. to replace characteristic functions with membership functions. This allows a more sufficient characterization of transiton states between different conformations and therefore leads to a better understanding of molecular dynamics. Furthermore, an indicator for the uniqueness of metastable fuzzy clusters is described.

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