Gyration-Radius Dynamics of Atomic Clusters and Polymers

Tomohiro Yanao

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Abstract

Large-amplitude collective motions of clusters and biopolymers are of great interest in chemistry and biophysics. For the true understanding of these high-dimensional dynamics, it is crucially important to find a small number of coarse variables that essentially dominate the collective motions of the system. In this talk, it is shown that the gyration radii (or moments of inertia) of molecules are good collective variables both in coarse-graining the high-dimensional dynamics and in clarifying the mechanism of collective motions. Equations of motion for the gyration radii are investigated based on the reduction theory and the hyperspherical coordinates. By averaging these equations of motion, we introduce a mean force potential along a reaction coordinate defined in the space of gyration radii. This mean force potential explains phase changes and branching ratios of structural isomerization dynamics of clusters and a prototypal polymer.