Investigations of imine-based unidirectional light-driven molecular motors by using *ab initio* multiple spawning dynamics

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Abstract

Light-driven molecular motors have raised broad interest due to their potential applications in material and biological systems, and the imine-based molecular motors are of particular interest due to their easy synthesis properties. [1-5] However, the mechanism of imine-based light-driven molecular motors is ambiguous due to the spatial and temporal resolution restriction of experimental equipment. In the past years, the photo-induced unidirectional isomerization mechanism of the molecular motors containing a C=N group was recognized as the rotation around the double bond on the excited state following the irradiation with light. In our work, we employ state-averaged complete active space self-consistent field (SA-CASSCF) electronic structure calculations combined with *ab initio* multiple spawning [6] (AIMS) dynamics to investigate the photo-isomerization mechanism of a series of imine-based unidirectional molecular motor and switches. The AIMS simulations reveal that the nonergodic and dynamic effect dominate the reaction mechanism, rather than several optimized geometries. New isomerization mechanism and guiding principles have been proposed, which would surely shed light on the improving the performance of molecular motor as well as the design of novel unidirectional molecular motors.

References

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