1. Record Nr. UNINA9910760297503321

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Titolo	Ab Initio Molecular Dynamics Analysis Based on Reduced-Dimensionality Reaction Route Map / / Takuro Tsutsumi
Pubbl/distr/stampa	Singapore : , : Springer, , [2023] ©2023
ISBN	981-9973-21-X
Edizione	[First edition.]
Descrizione fisica	1 online resource (123 pages)
Collana	Springer Theses Series
Disciplina	541.394
Soggetti	Molecular dynamics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di bibliografia	Includes bibliographical references.
Nota di contenuto	General Introduction -- Analysis of On-the-fly Trajectory based on Reaction Route Network -- 3. Visualization of Unique Reaction Route Map by Dimensionality Reduction Method -- 4. Projection of Dynamical Reaction Route onto Reduced-dimensionality Reaction Space -- 5. Theoretical Study of Excited-state Branching Reaction Mechanisms of -methyl-cis-stilbene -- 6. Visualization of Multi-state Potential Energy Landscape: A Case Study on Excited-state Branching Reaction of Stilbene -- 7. General Conclusion. .
Sommario/riassunto	This thesis proposes useful tools, on-the-fly trajectory mapping method and Reaction Space Projector (ReSPer), to analyze chemical reaction mechanisms by combining the reaction route map and the ab initio molecular dynamics. The key concept for the proposed tools is the Cartesian distance between pairwise molecular structures, and a practical procedure to get the optimal distance is introduced. The on-the-fly trajectory mapping method tracks the distance function between reference structures and molecular structures along the trajectory. Although this method provides fruitful insight into dynamic reaction behaviors, the visualization of reaction routes into a low-dimensional space is still challenging because of the multi-dimensionality. ReSPer successfully constructs a low-dimensional reaction space defined by mathematically-selected principal coordinates representing mutual distance relationships in the full-dimensional space. ReSPer also enables us to project trajectories into

the reaction space in the reduced dimension. In this thesis, these methods are applied to several reactions, including bifurcating and photochemical reactions, revealing dynamically-allowed reaction mechanisms. This thesis provides robust and versatile tools to elucidate dynamical reaction routes on the basis of the reduced-dimensionality reaction route map and will help control chemical reaction dynamics and select descriptors for machine learning. .