1. Record Nr. UNINA9910427687703321 Autore Liu Lai Chung Titolo Chemistry in action: making molecular movies with ultrafast electron diffraction and data science / / Lai Chung Liu Pubbl/distr/stampa Cham, Switzerland: ,: Springer, , [2020] ©2020 **ISBN** 3-030-54851-1 Edizione [1st ed. 2020.] Descrizione fisica 1 online resource (XX, 239 p. 110 illus., 106 illus. in color.) Springer Theses, Recognizing Outstanding Ph.D. Research, , 2190-Collana 5053 541.223 Disciplina Soggetti Stereochemistry Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Chapter1: Introduction -- Chapter2: Methods: Experimental Techniques Nota di contenuto and Data Science -- Chapter3: Ultrafast Structural Dynamics of (EDO-TTF)2X -- Chapter4: Photocyclization Dynamics of Diarylethene --Chapter5: Photoinduced Spin Crossover in Iron(II) Systems -- Chapter6: Future Work -- Chapter7: Conclusion. The thesis provides the necessary experimental and analytical tools to Sommario/riassunto unambiguously observe the atomically resolved chemical reactions. A great challenge of modern science has been to directly observe atomic motions during structural transitions, and while this was first achieved through a major advance in electron source brightness, the information content was still limited and new methods for image reconstruction using femtosecond electron diffraction methods were needed. One particular challenge lay in reconciling the innumerable possible nuclear configurations with the observation of chemical reaction mechanisms that reproducibly give the same kind of chemistry for large classes of molecules. The author shows that there is a simple solution that occurs

during barrier crossing in which the highly anharmonic potential at that point in nuclear rearrangements couples high- and low-frequency vibrational modes to give highly localized nuclear motions, reducing hundreds of potential degrees of freedom to just a few key modes. Specific examples are given in this thesis, including two photoinduced phase transitions in an organic system, a ring closure reaction, and two

direct observations of nuclear reorganization driven by spin transitions. The emerging field of structural dynamics promises to change the way we think about the physics of chemistry and this thesis provides tools to make it happen.