Record Nr. UNINA9910760268703321 Autore Louwerse Miranda **Titolo** Efficient Control and Spontaneous Transitions / / by Miranda Louwerse Cham:,: Springer Nature Switzerland:,: Imprint: Springer,, 2024 Pubbl/distr/stampa **ISBN** 3-031-40534-X Edizione [1st ed. 2024.] Descrizione fisica 1 online resource (123 pages) Springer Theses, Recognizing Outstanding Ph.D. Research, , 2190-Collana 5061 Disciplina 547.2 Soggetti Thermodynamics **Biophysics Biomolecules Biochemistry** Reaction mechanisms (Chemistry) Coding theory Information theory Condensed matter Molecular Biophysics **Reaction Mechanisms** Coding and Information Theory Phase Transitions and Multiphase Systems Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Nota di contenuto Chapter 1: Introduction -- Chapter 2: Theoretical Background --Chapter 3: Information Thermodynamics of Transition Paths -- Chapter 4: Multidimensional Minimum-Work Protocols -- Chapter 5: Connections between Minimum-Work Protocols and Transition Paths --Chapter 6 Conclusions. This thesis addresses deep questions that cut to the physical and Sommario/riassunto informational essence of central chemical quantities such as transition paths and reaction mechanisms and proposes fundamental new connections between transition-path theory, linear-response theory, nonequilibrium thermodynamics, and information theory. The author

investigates slow, energetically efficient driving protocols that drive a

system between conformations corresponding to endpoints of a reaction, aiming to find connections between principles of efficient driving and the spontaneous transition mechanism in the absence of driving. First, an alternative perspective of transition-path theory is developed that unifies it with stochastic thermodynamics to describe flows of entropy, energy, and information during the reaction. This also provides an optimization criterion for selecting collective variables. Next, protocols are designed which invert the magnetization of a 3x3 Ising model with minimal energetic cost, and it is determined that using multiple control parameters allows the system to be driven along a fast-relaxing pathway between reaction endpoints. Finally, the author compares these protocols with the spontaneous transition mechanism for magnetization inversion in the same Ising model, finding that designed protocols capture general features of the spontaneous mechanism and energetics given the constraints on the control parameters. This work represents a major step forward in our understanding of rare events and provides a basis for investigating the connection between efficient protocols and spontaneous transition mechanisms which can be further probed in a wider variety of systems.