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Physikalisches Kolloquium
Einladung

Physics Colloquium
Invitation

Monday, 14 February 2022

BE AWARE - ROOM CHANGE Lecture Hall 025/H2, 16:15

and via ZOOM

Topology, Landscapes and Biomolecular Energy Transport

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 www.nist.gov



While ubiquitous, energy redistribution remains a poorly understood facet of the nonequilibrium thermodynamics of biomolecules. At the molecular level, finite-size effects, pronounced nonlinearities, and ballistic processes conspire to produce behavior that diverges from the macroscale. Here, we show that transient thermal transport reflects macromolecular energy landscape architecture through both (i) the topological characteristics of the conformational ensemble and (ii) the nonlinear processes that mediate dynamics. While the former determines transport pathways via molecular contacts, the latter reflects the ruggedness of the landscape for local motion of atoms and molecular fragments. Unlike transport through small-molecule systems, such as alkanes, nonlinearity dominates over coherent processes at even quite short time- and length-scales. Our exhaustive all-atom simulations and novel local-in-time and space analysis, applicable to both theory and experiment, permit dissection of energy migration in biomolecules. The approach demonstrates that vibrational energy transport can probe otherwise inaccessible aspects of macromolecular dynamics and interactions that underlie biological function.

Host: Prof. Dr. Fedor Jelezko, Institute of Quantum Optics

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