Abstract Submitted
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Mixed quantum classical simulations of vibrational energy transport in alpha-helices[1] ANNE GOJ, ERIC BITTNER, University of Houston — We use mixed classical/quantum simulations to study the time dependence of an excitation of a C=O vibration on a 3-10 helix of α-Aminoisobutyric acid (AIB), a system which represents a test case for the formation of self-trapped vibrational excitation states on protein helices. Due to the inherent disorder in the system caused by the finite temperature and fluctuations in hydrogen bonding, the excitation tunnels randomly among C=O sites along the helix. Quantum forces are insufficient to establish a coherent relationship between the location of the excitation and the contraction of hydrogen bonds around this site. Our simulations indicate that the excitation frequently becomes localized on the end of the helix due to the defect in helical structure caused by unwinding. Our results generally do not support the existance of Davydov type solitons in biological helix systems under physiological conditions.

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