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Accession number:WOS:000307749100016

Title:Driving of a Small Solvated Peptide in the IR and THz Range-A Comparative Study of Energy Flow

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Source title:JOURNAL OF PHYSICAL CHEMISTRY B

Abbreviated source title:J PHYS CHEM B

Volume:116

Issue:33

Issue date:AUG 23 2012

Pages:10020-10025

Language:English

ISSN:1520-6106

Document type:Article

Publisher:AMER CHEMICAL SOC, 1155 16TH ST, NW, WASHINGTON, DC 20036 USA

Abstract:We present a comparative study of energy flow from a vibrationally excited solvated dialanine molecule to the surrounding water in the IR and THz range. We employ the driven molecular E dynamics (DMD) approach to investigate the energy flow from the solute molecule to water molecules. As a result, we find a more rapid and efficient energy flow from the solute to the water when exciting it THz modes compared to IR modes. Our results show a strong coupling of the low frequency mode of the solute and the water dynamics in the THz regime. In contrast, when exciting the IR modes of the solute, we find much more localized motions.

Number of references:22

Main heading:Chemistry

DOI:10.1021/jp3021358