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Accession number:20123315337832

Title>Note: Inverted time-ordering in two-dimensional-Raman-terahertz spectroscopy of water

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Source title:Journal of Chemical Physics

Abbreviated source title:J Chem Phys

Volume:136

Issue:23

Issue date:June 21, 2012

Publication year:2012

Article number:236101

Language:English

ISSN:00219606

CODEN:JCPSA6

Document type:Journal article (JA)

Publisher:American Institute of Physics, 2 Huntington Quadrangle, Suite N101, Melville, NY 11747-4502, United States

Abstract:The inverted time-ordered pulse sequence, in which the first coherence is generated by a direct THz excitation, while the switching of coherences is achieved by a Raman interaction, was studied. The dependence of the polarizability on the nuclear coordinates is expected to be more nonlinear compared to that of the dipole moment. The hybrid equilibrium-non-equilibrium approach introduced by Tanimura and co-workers is used to compute this response function from an all-atom MD simulation. An echo arises when a coherence dephases very quickly, and then rephases upon a second perturbation. Traces of a photon echo appear in simulations of 2D-Raman spectroscopy, but only when approximating the signal with instantaneous or quenched normal modes. It is concluded that indeed the inverted pulse sequence more sensitively measures the coupling between the various degrees of freedom of water.

Abstract type:(Edited Abstract)

Number of references:10

Main heading:Raman spectroscopy

Controlled terms:Physical chemistry - Physics

Uncontrolled terms:MD simulation - Normal modes - Nuclear coordinates - Photon echoes - Pulse sequence - Raman interactions - Response functions - Time ordering

Classification code:741.1 Light/Optics - 801.4 Physical Chemistry - 931 Classical Physics; Quantum Theory; Relativity - 932 High Energy Physics; Nuclear Physics; Plasma Physics - 933 Solid State Physics

DOI:10.1063/1.4729945

Database:Compendex

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