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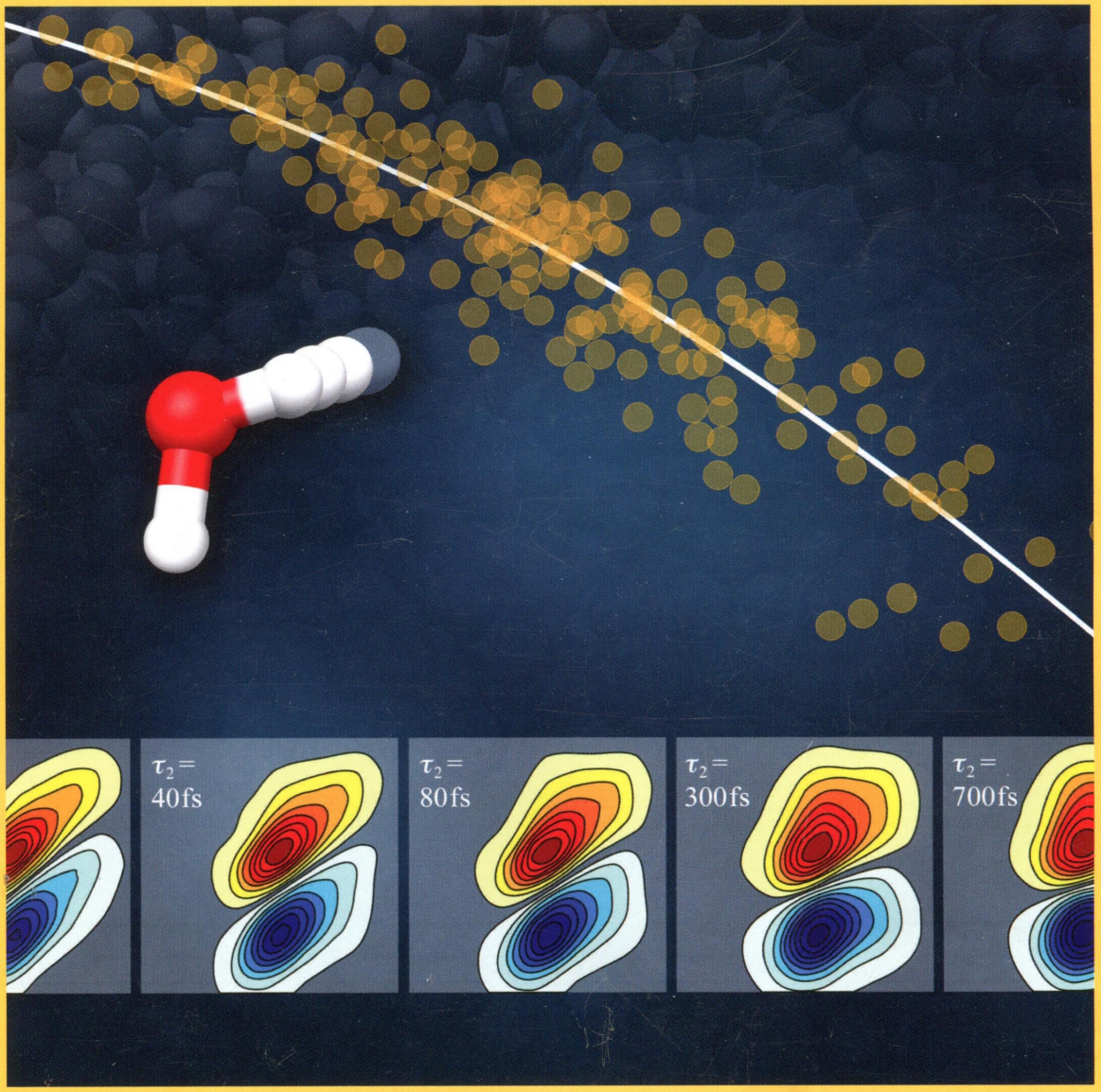

Spectroscopic Maps Allow the Calculation of 2D IR Spectra To Reveal the Dynamics of Liquid Water

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ON THE COVER: Spectroscopic maps allow the calculation of 2D IR spectra to reveal the dynamics of liquid water. Spectroscopic maps that relate the vibrational frequency of an infrared (IR) reporter to the electrostatic properties of its environment allow the calculation of vibrational spectra using classical molecular dynamics (MD) simulations. The simulations can then provide crucial molecular-level insights about the spectroscopic line shapes. In the background of the cover image is a snapshot from a MD simulation of liquid water. The water molecule in the foreground represents an HOD molecule whose OH vibration is reporting on the dynamics of the surrounding liquid. The scatter-plot data in yellow are OH stretch vibrational frequencies of aqueous HOD clusters extracted from an MD simulation plotted versus the electric field projected along the OH bond of interest. The white line is the quadratic fit to the data, which provides a map between the OH vibrational frequency and the electric field that is readily accessible in the simulation. Along the bottom of the image are 2D IR spectra of dilute HOD in D_2O calculated using spectroscopic maps. The 2D IR spectra reveal detailed information about the structure and dynamics of the liquid surrounding the OH reporter. The cover image was designed by Dr. Kristina E. Davis, a Visualization Specialist at the University of Notre Dame Center for Research Computing. This special issue was organized by Guest Editors Steven A. Corcelli, Brian B. Laird, Jeffrey G. Saven, and J. R. Schmidt.

SPECIAL ISSUE: JAMES L. SKINNER FESTSCHRIFT

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Special Issue Preface

Articles

Supporting Information available via online article