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标题: Two-dimensional-Raman-terahertz spectroscopy of water: Theory
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摘要: We discuss the hybrid 2D-Raman-THz spectroscopy of liquid water. This two-dimensional spectroscopy is designed to directly work in the low-frequency range of the intermolecular degrees of freedom. The information content of 2D-Raman-THz spectroscopy is similar to 2D-Raman or 2D-THz spectroscopy, but its experimental implementation should be easier. That is, 2D-Raman-THz spectroscopy is a 3rd-order nonlinear spectroscopy and as such completely avoids cascading of consecutive 3rd-order signals, which turned out to be a major difficulty in 5th-order 2D-Raman spectroscopy. On the other hand, it does not require any intense THz pump-pulse, the lack of which limits 2D-THz spectroscopy to the study of semiconductor quantum wells as the currently available pulse energies are too low for molecular systems. In close analogy to 2D-Raman spectroscopy, the 2D-Raman-THz response of liquid water is simulated from an all-atom molecular dynamics simulation, and the expected spectral features are discussed. (C) 2012 American Institute of Physics. [http://dx.doi.org/10.1063/1.3691601]
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