378. Title:Intermolecular electron density modulations in water and their effects on the far-infrared spectral profiles at 6 THz
Authors:Torii, Hajime (1)
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Abstract:The modulations in the electron density induced by molecular motions are analyzed theoretically for tetrahedrally hydrogen-bonded water molecules. Those modulations are represented as the electron density derivatives, and their forms are examined by the use of the one- and two-dimensional integrated plots. It is shown that intermolecular flux of electrons, called intermolecular charge flux, is induced by the molecular translation modes in water, leading to the infrared intensity at 6 THz. This means that the molecular translational and electronic motions are strongly coupled, and this coupling is observable through this vibrational band. A comparison is made with the case of the OH stretching mode. A method to incorporate this effect in spectral simulations based on classical molecular dynamics is also shown. These results provide a way to correct understanding of dynamics in, for example, aqueous solutions of biomolecules from analyses of their vibrational spectra in the terahertz frequency region. A general idea on how we can perform reasonable calculations and analyses of the vibrational spectral profiles of liquid systems is also discussed.