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New insights into the femtosecond-to-picosecond dynamics of liquid water from temperature dependence using terahertz spectroscopy studies and molecular dynamics simulations CHOLA REGMI, DEEPU GEORGE, SHENGFENG CHENG, NGUYEN VINH, Virginia Polytechnic Institute and State University — Water plays an active and complex role in sustaining life. The hydrogen bonds between the water molecules exhibit the unique physical properties that distinguish water from other molecular liquids. Nevertheless, there is little agreement regarding the femtosecond to picosecond relaxation dynamics of water. In response, we have used the state-of-the-art terahertz spectroscopy (frequency-domain and time-domain) and molecular dynamics simulation techniques to study the molecular relaxation of water at different temperatures in the femtosecond to picosecond time scale. We show that the two-Debye model is insufficient to explain the observed relaxation dynamics of water and our results on the terahertz dielectric relaxation of water are best described as the sum of three-Debye processes. We compute the time autocorrelation function of the dipole moment of water molecules at different temperatures with molecular dynamics simulations and compare the calculations with the experimental data.

Chola Regmi
Virginia Polytechnic Institute and State University

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