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Molecular dynamics behind the principle relaxation of water: Observation of inertia and memory effects[1] KOJI YOKOYAMA, A. JASON MCNARY, H. W. K. TOM, Department of Physics, University of California, Riverside, California 92521, ERIC SCHWEGLER, GIULIA GALLI, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94550 — We report an analysis of the single dipole to collective dipole moment time correlation function (TCF) calculated from the molecular dynamics simulations of liquid water at room temperature with a rigid and nonpolarizable TIP5P water model [1]. The single to collective dipole moment TCF is especially important because it allows us to investigate the local relaxation processes in a cluster of molecules and it can be directly related to the dielectric constant via the Fatuzzo-Mason equation. We have calculated the collective dipole moment associated with the first through fourth solvation shells and observed retarded relaxation processes for outer shells. We have also discovered a long-term and long-range rephasing process of about 40 ps involving more than 500 molecules. [1] M. W. Mahoney and W. L. Jorgensen, J. Chem. Phys. 112, 8910 (2000).

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