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Thermal diffusion and colored energy dissipation in hydrogen bonded liquids. RICCARDO DETTORI, Department of Physics - University of Cagliari (I), CLAUDIO MELIS, Department of Physics - University of Cagliari, MICHELE CERIOTTI, Ecole Polytechnique Federale de Lausanne (CH), DAVIDE DONADIO, Department of Chemistry - UC Davis (USA), LUCIANO COLOMBO, Department of Physics - University of Cagliari (I) — H-bonded liquids show a manifold energy dissipation dynamics due to: strong directionality of H-bonds and complexity of their network. This affects both thermal diffusion and energy dissipation mechanisms in pump-probe spectroscopy experiments. By nonequilibrium molecular dynamics (MD) simulations we investigate such phenomena in liquid methanol. While heat transport is studied by approach-to-equilibrium MD, energy dissipation is investigated by making use of a novel Generalized Langevin Equation (GLE) colored noise thermostat, which can generate a non-equilibrium frequency-resolved dynamics by using a correlated noise. The colored thermostat can thermally excite a narrow range of vibrational modes, typically the stretching mode of the OH involved in H-bonding, leaving the other degrees of freedom at the equilibrium temperature. The energy dissipation is then observed as a function of time, by probing the excitation decay and the energy transfer to other modes. In particular, by monitoring in time the different contributions to the potential energy of the system, we evaluate how energy is transferred from the excited mode to other modes of the nearby molecules and provide understanding on the dynamics of H-bonded liquids, as resulting from current experimental investigations

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