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Nuclear quantum effects using selective mode excitation in water

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— Recently, Ceriotti et. al. [1] introduced a comprehensive framework to use a custom-tailored Langevin equation with correlated-noise in the context of MD simulations. One of the interesting applications of these thermostats is that, such a framework can be used to selectively excite normal modes whose frequency falls within a prescribed, narrow range [2]. The general idea of this work is to understand whether, the selective excitation of modes in some systems like water is enough to reproduce the necessary nuclear quantum effects at a given temperature. Ceriotti et. al has also implemented their colored noise thermostat (Langevin) to the PIMD of TIP4P/F model [3]. In this work we study how the TIP4P/f responds to the selective mode excitation using the delta-thermostats. We apply this delta thermostat to the molecular dynamics of TIP4P/F [4] water force field, a model explicitly fitted with the lack of zero point ionic vibrations. TIP4P/F provides us an ideal platform to study the effect of selective mode excitation on water. We address the question of whether selective mode excitations are enough to generate the nuclear quantum effects in water. This work will also provide a way to identify the dominant modes for which the quantum effects are important. [1] Chem. Theory Comput.6, 1170 (2010) [2] Proc. Comp. Sci. 1, 1601 (2010), [3] J. Chem. Phys. 131, 024501 (2009), [4] J. Chem. Phys 133, 124104 (2010).

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