APPLICATIONS OF PATH INTEGRAL LANGEVIN DYNAMICS TO WEAKLY BOUND CLUSTERS AND BIOLOGICAL MOLECULES

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We present the use of path integral molecular dynamics (PIMD) in conjunction with the path integral Langevin equation thermostat[a] for sampling systems that exhibit nuclear quantum effects, notably those at low temperatures or those consisting mainly of hydrogen or helium. To test this approach, the internal energy of doped helium clusters are compared with white-noise Langevin thermostatting and high precision path integral monte carlo (PIMC) simulations. We comment on the structural evolution of these clusters in the absence of rotation and exchange as a function of cluster size. To quantify the importance of both rotation and exchange in our PIMD simulation, we compute band origin shifts for $(He)_N$-CO_2 as a function of cluster size and compare to previously published experimental and theoretical shifts[b]. A convergence study is presented to confirm the systematic error reduction introduced by increasing path integral beads for our implementation in the Molecular Modelling Toolkit (MMTK) software package. Applications to carbohydrates are explored at biological temperatures by calculating both equilibrium and dynamical properties using the methods presented.

[a] M. Ceriotti, M. Parrinello, and D. E. Manolopoulos, J Chem Phys 133, 124104.
[b] H. Li, N. Blinov, P.-N. Roy, and R. J. L. Roy, J Chem Phys 130, 144305.