

# Simulating steady state spectra of acrolein while accounting Nuclear Quantum Effects

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This study investigates the photoabsorption cross-section spectra of the atmospheric volatile organic compound acrolein in both gas and aqueous phases by incorporating Nuclear Quantum Effects (NQE) at the cost of classical molecular dynamics. Using adaptive Quantum Thermal Bath (adQTB) method the zero point energy leakage (ZPEL) is treated, which has plagued standard Quantum Thermal Bath (QTB) dynamics. The spectroscopic results obtained are in excellent agreement with quantum molecular dynamics (Path Integral MD) method, experimental observation and previous works on photoabsorption spectrum of acrolein molecule. The adQTB approach was able to capture weak  $n \rightarrow \pi^*$  transitions and broadening in the gas phase, as well as the blue shift and reduced peak intensity due to solvent effects in the aqueous phase. The adQTB method is shown to perform - if not better - at par with PIMD in gas and solvent phase while being much superior to classical MD and standard QTB method particularly for solvated systems. This work shows that using adQTB method, it is possible to overcome the ZPEL and use QTB based method to study spectroscopic properties.

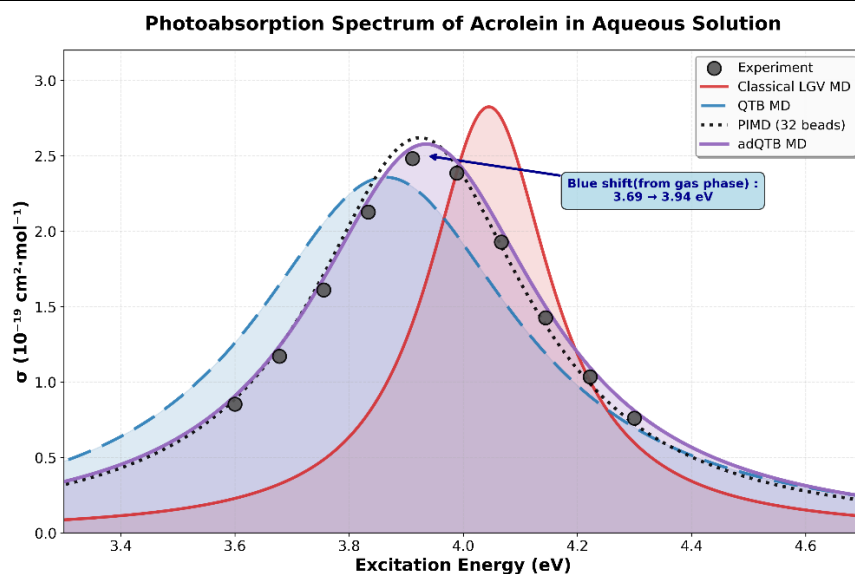


Figure: The figure represents the adQTB spectrum as captured for the acrolein in solvent phase. We see the blue shift captured compared to gas phase calculations and the solvent spectral properties captured by adQTB method which agrees with experimental and PIMD calculations.

[1] M. Dhiman *et al* JPCA (In Review)

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