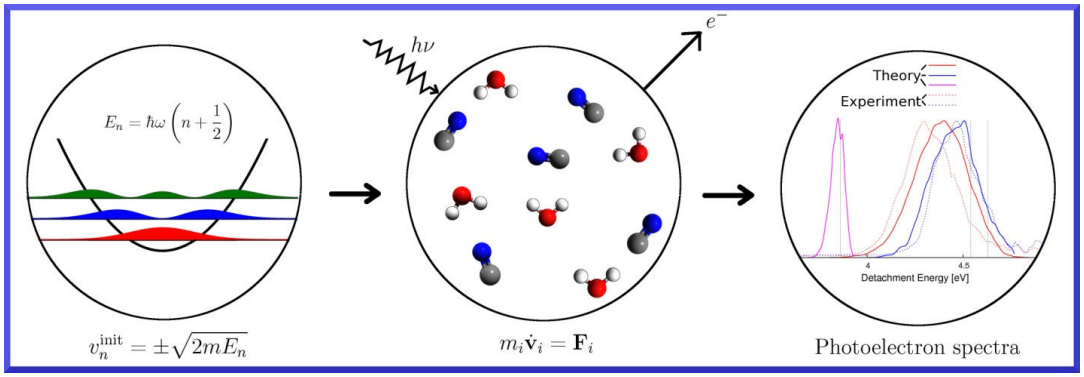
A Quantum Leap Into the Future of Chemistry

What's New in Q-Chem

Quasiclassical Trajectory Molecular Dynamics (QCT-MD)

Developers: Daniel Lambrecht, Martin Head-Gordon

QCT-MD is a cost-effective way of incorporating zero-point motion into otherwise classical simulations. This feature puts vibrational energy into each mode during an MD simulation. This can lead to a more realistic sampling of the potential energy surface and thus improve the description of anharmonic effects and of spectral features such as peak widths. QCT-MD is particularly effective for any type of MD simulation where vibrational effects are important, e.g. for simulating IR or photoelectron spectra.



The above scheme explains the basics of a QCT-MD photoelectron spectra simulation: First, the initial velocities are chosen according to the energy of a harmonic oscillator. The system is then propagated using classical Newtonian dynamics. We then calculate vertical detachment energies (VDEs) along the trajectory and obtain the simulated spectrum as a (weighted) histogram of the VDEs.

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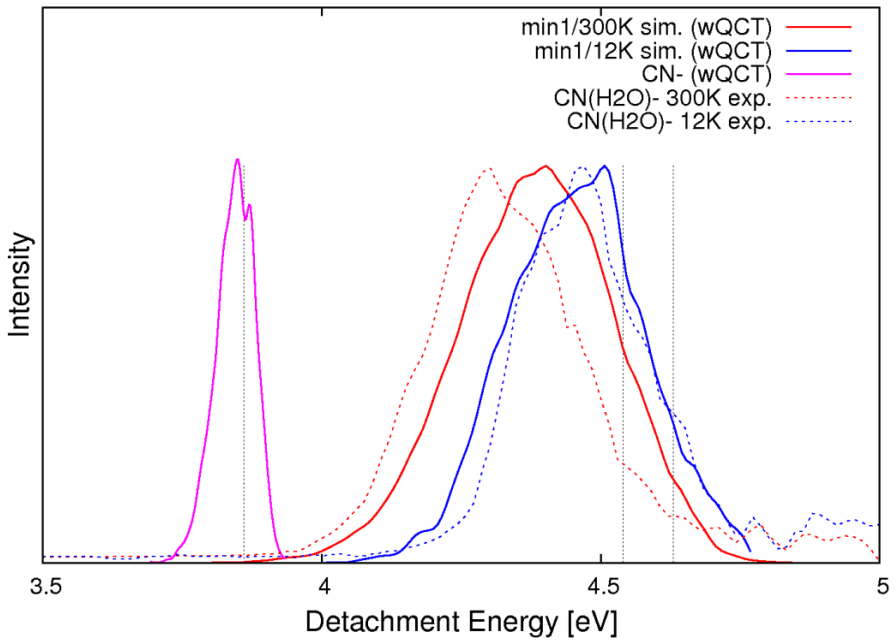
Quasiclassical Trajectory Molecular Dynamics (QCT-MD) (continued)

Below we compare the final results: the simulated and the experimental photoelectron spectra for an aqueous cluster of cyanide. The simulated peak widths and positions agree reasonably well with experiment, even at low temperature. In contrast to that, purely classical MD yields zero (!) peak width at low temperature.



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Quasiclassical Trajectory Molecular Dynamics (QCT-MD) (continued)

Daniel Lambrecht

Publications: Daniel Lambrecht, Martin Head-Gordon, "[insert article title here]"

J.Phys. Chem. A, [submitted-insert ref. here]

Faraday Discuss., [submitted-insert ref. here]

For more information on how to use this feature, refer to the Q-Chem Manual, Section ____:

For see more new features, visit:
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