Using Diffusion Monte Carlo to Decode Signatures of Large Amplitude Motions in Molecules and Ions

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Diffusion Quantum Monte Carlo has proven to be a powerful technique for studying a broad array of chemical systems, focusing on either the quantum nature of vibrations or the electronic structure. This talk will focus on recent developments in our group that have allowed us to explore rotation/vibration states of highly fluxional molecules and clusters, like H5+, CH5+, protonated and neutral water clusters with a focus on the physical insights that can be obtained by such studies. Two specific advances have been the development of hybrid approaches for studying rotation-vibration excited states of such molecules in which the vibrational degrees of freedom are propagated in coordinate space while the rotational degrees of freedom are propagated in state space. We will also discuss general approaches that allow us to perform ground and excited state calculations in arbitrary coordinates.

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