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Monte Carlo / Quantum Monte Carlo study of water clusters SHIV UPADHYAY, JEFFRY D. MADURA, Duquesne University — Water plays an important role in many physical, chemical and biological processes, however a complete description of the complex behavior of water from first principles does not exist. Much of the chemically relevant properties of water are a results of the hydrogen bond. The most common computational approach to exploring the atomic and electronic degrees of freedom of an aqueous system is Born-Oppenheimer molecular dynamics using density functional theory. The hydrogen bond is an interaction dominated by electrostatics dispersion, however dispersion plays an important role, which density functional theory fails to describe. Quantum Monte Carlo has been shown to perform well on hydrogen bonding systems, and more importantly on systems with dispersion. Here, we present our work on a Monte Carlo / Quantum Monte Carlo method to study the thermodynamic properties of water clusters.

Shiv Upadhyay
Duquesne University

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