

Abstract Submitted  
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**Studies of energetics and spectroscopy of water clusters: size evolution and connections to the spectrum of liquid water** ANNE MCCOY, Department of Chemistry and Biochemistry, The Ohio State University — In this talk, I will focus on recent work in our group on water clusters. The first part will focus on interpreting the origins of the band at  $2100\text{ cm}^{-1}$  in the absorption spectrum of liquid water. Based on its frequency, the band has long been assigned to a combination band involving intramolecular bend vibration and intermolecular librations. The intensity arises from changes in the transition moment for the HOH bend as the low-frequency librations form and break intermolecular hydrogen bonds. In the second part we investigate approaches for using Diffusion Monte Carlo for studying the zero-point averaged vibrational structure of water clusters. The weak coupling between the inter- and intra-molecular degrees of freedom makes these challenging systems for DMC. Approaches taken and insights gained from this work will be described.

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