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Abstract for an Invited Paper for the MAR17 Meeting of the American Physical Society

## Theoretical and Computational Studies of the IR Spectra of Small Water and Protonated Water Clusters JOEL BOWMAN, Emory University

Recent spectroscopic measurements of IR spectra of water and protonated water clusters, from the from the Havenith and Johnson groups, respectively, present major challenges to theory. These include rigorous calculations of these spectra, using high-level ab initio potential and dipole moment surface and simple models to provide insights into both the experiments and the calculations. I will present our progress on both accounts, focusing on intermolecular and bending vibrational of the water clusters and the complex proton stretch modes in protonated water clusters. For the latter, the central role of the Zundel potential will be emphasized.