THEORETICAL RESULTS FOR $(H_2O)_nH^+$ AND $(H_2O)_n$: QMC FOR $H_5O_2^+$, GRAPH THEORETICAL ENUMERATION OF DISTINCT HYDROGEN-BONDED ARRANGEMENTS, COMPACT TO EXTENDED PHASE TRANSITIONS IN $(H_2O)_nH^+$

SHERWIN J. SINGER, LARS OJAMÄE and ISAIAH SHAVITT, *Department of Chemistry, Ohio State University, Columbus, OH 43210.*

Our recent progress in the study of protonated and neutral water clusters, $(H_2O)_nH^+$ AND $(H_2O)_n$, is reviewed. Both variational and diffusion Monte Carlo calculations have been performed, leading to a prediction of the fundamental frequency for motion of the central proton in $H_5O_2^+$. *Ab initio* electronic structure calculations suggest this absorption feature will be intense. Extensive Monte Carlo simulations of larger hydrated proton clusters indicate there is a transition between compact and extended phases. Local minima of the potential energy surface for $(H_2O)_nH^+$ AND $(H_2O)_n$ are studied. The number of topologically distinct hydrogen-bonded arrangements can be enumerated using graph theory, leading to a prediction of the number of distinct local minima of the potential energy surface in compact geometries, including dodecahedral clathrate structures.