Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Structure of Water Clusters in the Presence of Acidic Defects

CAITLIN BRESNAHAN, REVATI KUMAR, Louisiana State Univ - Baton Rouge

— Water clusters play an important role in atmospheric processes such as gas-liquid nucleation. The presence of acidic defects in these clusters can change the free energy profile of nucleation. Molecular level insight into gas-liquid nucleation events is often not possible via experimental methods, necessitating the use of computational models. Modeling these acidic water clusters is challenging due to Grotthuss proton shuttling, the mechanism by which an excess proton hops over multiple water molecules connected via the hydrogen bond network. In order to gain an accurate molecular level interpretation of these processes and account for the physics of proton transfer and delocalization in these hydrogen bonded water clusters, reactive molecular models are required. We are developing a reactive model, based on the empirical valence bond approach, parameterized on ab initio data, to model water clusters with acidic defects like HCl. This model will be incorporated into Aggregation-Volume-Bias Monte Carlo to study nucleation in the presence of acidic defects in hydrogen bonded water clusters. The development of the model along with the results on the hydrogen bond structure and the solvation of the acidic defects, as a function of cluster size, will be presented.

Caitlin Bresnahan
Louisiana State Univ - Baton Rouge

Date submitted: 10 Nov 2016 Electronic form version 1.4