



ALEXIS J. LEE
UNIVERSITY OF NEW ORLEANS
COMPUTATIONAL AND THEORETICAL CHEMISTRY
504.388.6729 · ALEXISJLEE@YAHOO.COM · AJLEE1@MY.UNO.EDU

Authors: Alexis J. Lee and Steven W. Rick

Title: New methods to treat charge transfer at the air/water interface—Discrete Charge Transfer (DCT)

Abstract: Charge transfer in hydrogen-bonding systems, or asymmetrically-bonded systems, has been shown to contribute 20-40% to the interaction energy between molecules, depending on the partitioning method used. The asymmetry between molecules of the water–water dimer, in particular, leads to a transfer of a small, but significant, amount of charge ($-0.02e$) from the hydrogen-bond acceptor molecule back to the hydrogen-bond donor. Recently developed are two new computational methods for treating charge transfer associated with the formation of a hydrogen bond, which may be easily parameterized and applied to water potentials. Discrete charge transfer (DCT) has been parameterized for both non-polarizable and polarizable potentials, TIP4P+DCT and TIP4P-FQ+DCT. Both models have been applied to investigate the effects of charge transfer at the air/water interface.