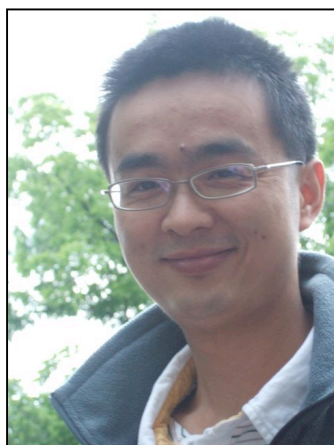


# Dynamics of hydrogen bonding in neutral, excited and cationic states

Wednesday, November 13, 2013  
2:00 p.m. Room 9341



**Dr. Quanli Gu**  
*Research & Development*  
*Basic Science Department*  
*R. J. Reynolds Company*

9-hydroxy-9-fluorene carboxylic acid (9HFCA), an analog of glycolic acid, is found to be a good substrate for spectroscopic studies of multiple H bonds in water and carboxylic acid clusters. Infrared and ultraviolet spectra of these complexes show rich information about the nature of H-bonding interactions in neutral, excited and cationic states. Density functional calculations reveal the subtle relationship of anticooperative and cooperative interactions among intra and inter molecular hydrogen bonds. Moreover NBO analysis shows how the charge transfer shows up even in more subtle side effects of competitive donor-acceptor H-bonding.