



Hosted by Mike Haley

Dept. of Chemistry and Biochemistry  
Organic/Inorganic Seminar Series

**Judy I-Chia Wu**

University of Houston

**Wednesday, October 31, 2018**

Coffee reception at 3 pm, 377 KLA,

Seminar at 3:30 pm, 331 KLA

## ***Aromaticity-Modulated Hydrogen Bonding***

Abstract: Aromaticity and hydrogen bonding interactions are traditionally considered to be largely separate chemical concepts. We show, however, that their reciprocal effects are significant and provide insights to understanding puzzling problems pertaining to molecular recognition, assembly, proton-coupled electron transfer, and even enzyme catalysis. Evidence based on computational quantum chemical calculations and experiments document the effects of such aromaticity-modulated hydrogen bonding (AMHB). According to the AMHB relationship, hydrogen-bonding interactions that increase cyclic  $4n+2$   $\pi$  electron delocalizations (enhanced aromaticity) in heterocycles are strengthened, while those that decrease (reduced aromaticity) cyclic  $4n+2$   $\pi$  electron delocalization are weakened. We also show that, at specific excited states, these trends *reverse* following Baird's Rule for excited-state aromaticity ( $4n$   $\pi e$ ) and excited-state antiaromaticity ( $4n+2\pi e$ ). Representative examples will be discussed.