Halogen bonding (XB) is defined as the non-covalent interaction formed between halogen atom X and a heteroatom A. Due to its unique features, XB has found extensive use in medicinal, supramolecular, and materials chemistry. In this way, XB has adopted an exceptional role among the noncovalent interactions. Despite the many investigations on XB carried out so far, there is no quantitative assessment on its intrinsic bond strength and a detailed description of its nature. We have systematically analyzed XB in dependence of X and A. For the quantification of the intrinsic strength of the X ... A interaction we have used new quantum chemical tools, which in combination with Coupled Cluster calculations provide for the first time a direct insight into the nature and strength of halogen bonding. Calculated binding energies between 1 and 45 kcal/mol reflect the large variation in XB. An outlook is given on how to utilize XB as a building block for crystal engineering, materials science, and drug design.

**CBC SEMINAR ANNOUNCEMENT**

**Professor Elfi Kraka**  
Southern Methodist University  

*Nature and Intrinsic Strength of the Halogen Bond*

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Date: 1st June 2016 (Wednesday)  
Time: 2:30pm – 3:30pm  
Venue: SPMS Research & Graduate Studies Office Conference Room  
Host: Asst Professor Hajime Hirao