In Silico Design of Halogen-Bonding-Based Catalysts

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The strong, specific and directional halogen bond (XB) is an ideal *supramolecular synthon* in crystal engineering, rational catalyst, and drug design. These attributes have attracted strong growing interest in halogen bonding in the past decade and led to a wide range of applications in materials, biological and catalysis applications. In this presentation, we will report our application studies on XB to catalyst design. For catalysis application, various experimental groups have exploited the XB mode of activation in designing halogen-based Lewis acids in accelerating and controlling organic reactions. Computational investigations are well suited to mechanistic understanding, rational XB catalyst design and study of intermediates that are unstable to be observable experimentally.

Preorganization is a common strategy to align halogen bond (XB) donors to form two or more halogen bonds simultaneously. In this talk, we reported our strategy to preorganize halogen bond donors and *in silico* design of new catalytic motifs. The structures of our designed XB catalysts have multiple XB donor moieties connecting optimally via covalent bonds. We will highlight *in silico* computational design on two types of XB based catalyst, namely tridentate triaryl benzene and bidentate thiourea-like XB donors. Density Functional Theory (DFT) calculations predicted that our designed catalysts may catalyze important organic reactions, such as Diels-Alder reaction, Claisen rearrangement, cope-type hydroamination and Michael addition.