☆EVENT　カデット後援セミナー☆

2014 年 1 月 8 日(水)　 14:40～16:10

大阪大学 理学研究科 理学部 D 棟 3 階 D307 教室

講師をお招きしてセミナーを開催しました

講師名：Prof. Miklos Kertesz

講師所属： Georgetown University

講演タイトル： Pancake bonding vs. π-π stacking: overview and interpretations

『新しい共有結合の概念に関する最新の研究内容について』

Abstract：In highly conducting organic crystals neighboring radicals display uniquely short contacts due to the overlap of the singly occupied molecular orbitals, SOMOs. These unusual intermolecular bonds occur between (1) conjugated molecules with delocalized π-electrons, and are further characterized by (2) good face to face π stacking overlap and (3) shorter than van der Waals (vdW) contact distances. These aggregates differ qualitatively from ordinary π stacking that occur between closed shell systems such as between DNA base pairs. This intermolecular interaction (termed “pancake bonding” after Mulliken and Person) has these further characteristics: (4) the binding energy can be significantly larger than typical vdW interactions, (5) intermolecular orbital overlap is important and dictates preferred relative packing by maximizing SOMO-SOMO overlap, (6) there are low-lying triplet and singlet excited states. These systems are characterized by low lying triplets in dimers and more complex magnetism other aggregates, such as chains. This type of interaction has wide ranging applications as organic conductors and magnetic materials. Another application of pancake bonding is in reaction mechanisms: transition structures and intermediates can be stabilized by

pancake bonds. Much has been learned about pancake bonding using experimental methods that include structure determination by single crystal X-ray diffraction, conductivity, ESR and magnetism, and other spectroscopies. Additionally, computational methods have been applied for interpretative and predictive purposes. This talk summarizes computational results obtained at Georgetown University.

The pancake bonding problem is theoretically challenging because the multireference (diradicaloid) character of the ground state appears together with significant dispersion that requires the inclusion of a large number of configurations. We discuss the application of wave function methods (MR-AQCC, [4]) and various density functional theory (DFT) approaches that include long-rage or dispersion terms. Although vdW interaction is an essential component of pancake interaction, it is significantly different from vdW interaction. We explore the limits of pancake bonding: which might be the strongest/shortest pancake bond?

[1] Tian, Y.-H.; Kertesz, M. J. Am. Chem. Soc., 132, 10648 (2010).
[2] Beneberu, H. Z.; Tian, Y.-H.; Kertesz, M. Phys. Chem. Chem. Phys. 14, 10713 (2012).
[3] Tian, Y.-H.; Kertesz, M. Chem. Comm. 46, 4282 (2010).
[4] Cui, Z.-h.; Lischka, H.; Mueller, T.; Plasser, F.; Kertesz, M. ChemPhysChem (accepted, 2013 VIP).

＜主催した先生から＞

Kertesz 教授は、理論計算を用いたπ電子系化合物の電子状態研究で著名な成果を挙げておられます。本講演会では、開殻化合物の二量体内に働く相互作用に関する最近の研究成果を紹介していただき、新しい共有結合の概念について議論を行いました。

（久保孝史教授）