Frontier Chemistry Center
フロンティア化学教育研究センター

講演会

演 題：**Exploring the Magnetism of Hexagonal Perovskites**

講 師：**Patrick Woodward 先生**
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日 時：2025 年 10 月 1 日（水）16:00~16:55

場 所：北海道大学工学部 材料・化学系棟大会議室（MC526）

共 催：FCC, JPEAKS

要 旨

Hexagonal perovskites share the ABX3 stoichiometry and cation coordination environments of the more widely studied “cubic” perovskite family, but unlike their cubic counterparts, hexagonal perovskites feature face-sharing linkages between metal-centered octahedra. When transition-metal ions occupy these sites there can be sufficient overlap of d-orbitals on neighboring metals to form metal-metal bonds. In such cases the clusters of face-sharing octahedra can be treated as having an electronic structure akin to a molecule. In this talk I will discuss the structure, bonding, and magnetism of various oxide and chloride hexagonal perovskites. Depending on the identity of the cations that occupy the octahedral holes and the nature of the anion, various degrees of metal-metal bonding occur. Furthermore, by controlling the composition we can magnetically isolate the face-sharing clusters to accentuate the molecule-like behavior. In such instances the frustrated triangular network that is characteristic of hexagonal perovskites can lead to exotic low temperature magnetic phenomena, such as quantum spin liquids. Alternatively, we can the face-sharing clusters can be linked by octahedra containing magnetic ions, in which case strong superexchange interactions lead to high-temperature magnetic ordering.

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