第185 回フロンティア材料研究所学術講演会

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9月9日（月） 13時30分～ J1棟809号室

演 題 ： Vacancy-ordered Double Perovskites: A route to host unconventional Magnetism

Vacancy-ordered halide double perovskites (DPs) hosting 4d/5d transition metals have emerged as a distinct platform for investigating unconventional magnetism arising out of the interplay of strong atomic spin-orbit coupling (SOC) and Coulomb interactions. Focusing on the d2 system Cs2WCl6, our ab initio electronic structure calculation reveals very narrow electronic bands, fulfilling the necessary condition to realize exotic orders, like multipolar magnetism. While multipolar magnetism has been proposed and actively investigated in certain cubic 5d2 osmate double perovskites, such as Ba2MgOsO6 and Ba2ZnOsO6, conclusive evidence of multipolar order in these 5d2 oxide DPs is lacking.[1] Vacancy-ordered DPs in which the second B′ site is vacant, resulting in isolated BX6 octahedra bound electrostatically by A-site cations appear to be an ideal platform to investigate unconventional forms of magnetism. Our study involving solution of the many-body spin-orbit coupled single-site problem by exact diagonalization show that the multiplet structure of Cs2WCl6 hosts ground non-Kramers doublets on W, with vanishing dipole moment and a small gap to an excited magnetic triplet. Our work provides the rationale for the observed strong deviation from the classic Kotani behaviour in Cs2WCl6 for the measured temperature dependence of the magnetic moment. The non-Kramers doublets on W exhibit non-zero quadrupolar and octupolar moments, and our calculated two-site exchange supports the dominance of inter-site octupolar exchange over quadrupolar interactions. We predict ferro-octupolar order with Tc~5 K, which may get somewhat suppressed by quantum fluctuations and disorder; this could be tested in future low-temperature experiments.[2]

[1] S Voleti, K Pradhan, S Bhattacharjee, T Saha-Dasgupta, A Paramekanti, npj Quantum Materials 8 (1), 42 (2023).
[2] Koushik Pradhan, Arun Paramekanti, and Tanusri Saha-Dasgupta, Phys. Rev. B 109, 184416 (2024)

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