# Effective theory for novel Kitaev candidate $OsCl_3$

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**Keywords: Mott insulators, Magnetic orderings**

Kitaev model is a theoretical model in which spin-1/2 moments on a honeycomb lattice are coupled via bond-dependent anisotropic Ising-type interactions, and its exact solution is known to realize a spin liquid state [1]. The Kitaev spin liquid is expected to have applications in quantum computation, and the search for candidate materials has therefore attracted considerable attention. In realistic materials, the Kitaev-type interaction arises from electron hopping mediated by ligand ions [2]. One of the most promising candidates is $RuCl_3$, which is described as an effective spin-1/2 system due to strong spin-orbit coupling. However, zigzag magnetic ordering emerges at low temperatures due to non-Kitaev interactions [3]. As another candidate material, $Os_xCl_3$, which forms a triangular lattice structure with vacancies, has been synthesized, and no magnetic ordering has been observed down to low temperatures [4]. Nevertheless, the observed disordered behavior may originate from short-range magnetic order associated with the defects. More recently, the high-pressure synthesis of $OsCl_3$ has been reported in three structures: an undistorted honeycomb lattice ($P\bar{3}1c$), a distorted honeycomb lattice ($C2/m$), and a hyperhoneycomb lattice (*Fddd*) [5].

In this study, we aim to reveal the magnetic properties of $OsCl_3$ using first-principles calculations based on the reported crystal structure. First, we construct the multiorbital Hubbard model using Quantum ESPRESSO, Wannier90, and RESPACK [6]. We then derive a localized effective model in the strong-coupling limit based on perturbation theory.

For the two honeycomb structures, $P\bar{3}1c$ and $C2/m$, the resulting interactions are similar, and mean-field theory favors an in-plane antiferromagnetic zigzag state in both cases. Spin-wave theory, however, finds a larger reduction of the ordered moment in $P\bar{3}1c$ than in $C2/m$, indicating stronger quantum fluctuations in the former structure. For the hyperhoneycomb *Fddd* structure, we obtain a skew-zigzag state with a weak ferromagnetic component. In the presentation, we will discuss the magnetic ordering state and its instability based on mean-field theory and spin-wave theory. Furthermore, we will present a computational package for spin-orbital Mott insulators based on perturbation theory, which we have recently developed [7, 8].

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