Abstract

In the search for quantum spin liquids, candidate materials for the Kitaev model and its extensions have been intensively explored during the past decade, as the models realize the exact quantum spin liquids in the ground state. Thus far, insulating magnets in the low-spin d^5 electron configuration under the strong spin-orbit coupling have been studied for realizing the Kitaev-type bond-dependent anisotropic interactions between the spin-orbital entangled Kramers doublets. To extend the candidates, here we investigate the systems in a high-spin d^7 electron configuration, whose ground state is described by the spin-orbital entangled Kramers doublet. By the second-order perturbation in terms of the t_{2g}-t_{2g} and t_{2g}-e_g hoppings, we show that the effective spin model possesses the anisotropic Kitaev interactions as well as the isotropic Heisenberg ones. While the Kitaev interaction is always ferromagnetic, the Heisenberg interaction can become either ferromagnetic or antiferromagnetic depending on the Coulomb interactions and the crystalline electric fields. We also derive the effective model for the low-spin d^5 electron configuration within the same perturbation scheme, in which the Kitaev interaction becomes both ferromagnetic and antiferromagnetic, while the Heisenberg one always ferromagnetic. Referring to the previous study for the Kitaev-Heisenberg model, we find that the quantum spin liquid phase exists in the reasonable parameter region in both d^7 and d^5 cases, while the former has a richer structure of the phase diagram. We discuss the advantages of the d^7 case in comparison with the d^5 case. Our results indicate that the high-spin d^7 state provides another platform for the Kitaev-type quantum spin liquid.