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First-principles study on electronic properties of the pyrochlore oxide Cd2Os2O7[1] HIROSHI SHINAOKA, NRI,AIST, TAKASHI MIYAKE, SHOJI ISHIBASHI, NRI, AIST — The pyrochlore oxide Cd2Os2O7 is one of 5d pyrochlore oxides in which the interplay of geometrical frustration, electron correlation, and spin-orbit coupling is expected. This compound exhibits a metal-insulator transition at 227 K, below which the emergence of a magnetic order has been suggested by experiments. Despite extensive studies for over thirty years, however, the nature of the low-temperature phase remains to be clarified. We depict the ground-state phase diagram based on the LSDA+U method (LSDA denotes local spin density approximation). We find that the all-in/all-out non-collinear magnetic order is stable in a wide range of U. We show that the easy-axis anisotropy arising from the spin-orbit coupling plays a significant role in stabilizing the all-in/all-out magnetic order. A pseudo gap extending up to high energy is found to appear near a continuous metal-insulator transition between an antiferromagnetic metallic phase and an antiferromagnetic insulating phase. Based on the computed results, we discuss possible origins of peculiar low-temperature properties observed in experiments.

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