Describing the magnetic structure and origin of band gap on Ba_2CuOsO_6 system; density functional theory approach

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We examine the magnetic structure and origin of band gap opening for Ba_2CuOsO_6 by extracting spin exchange interaction and by adopting spin-orbit coupling effect. The ordered double-perovskites Ba_2CuOsO_6which consist of 3d and 5d transition-metal magnetic ions (Cu^{2+} and Os^{6+}, respectively) is magnetic insulators; the magnetic susceptibilities of Ba_2CuOsO_6 obey the Curie-Weiss law with dominant antiferromagnetic interactions and the estimated Weiss temperature is -13.3 K. Solid-state osmium oxides can exhibit a variety of magnetic and electronic phenomena associated with their electron correlation. There are two important issues on solid-state osmium oxides; one is origin of band gap inducing metal to insulator transition. Other one is variety of oxidation state of Os ion.This wide spectrum of oxidation state of Os atom on osmium compounds is directly attributable to a large a spatial extension of Os 5d orbital. From the results of density functional study, the spin exchange interaction between Cu atoms is mainly responsible for antiferromagnetic ordering on Ba_2CuOsO_6 system. To describe the magnetic insulating states of Ba_2CuOsO_6, it is necessary adopting anelectron correlation effect as well as spin-orbit coupling effect.