Abstract Submitted
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Examination of the magnetic structure of Cs_2CuCl_4 by first principles DFT calculations[1] CHANGHOON LEE, Department of Chemistry, NCSU, JINHEE KANG, Department of Chemistry, Wonkwang University, S. Korea, MIKE WHANGBO, Department of Chemistry, NCSU — The spin-1/2 Cu^{2+} ions of Cs2CuCl4 have a 3D arrangement, but the magnetic properties of Cs2CuCl4 are mainly described by a quasi-2D triangular antiferromagnetic layer model. To understand why the 3D arrangement of $(CuCl4)^{2-}$ ions leads to a 2D magnetic behavior, we evaluated the various spin exchange interactions between adjacent $(CuCl4)^{2-}$ ions by performing DFT calculations. Our results show that the 6p orbitals of Cs^+ participate in the spin exchange interaction through the Cl?Cs?Cl bridges if the two $(CuCl4)^{2-}$ ions have a symmetric arrangement and if the Cl?Cs?Cl bridges are symmetric, and that the frustrated 2D triangular antiferromagnetism originates from this selective participation of the Cs 6p orbitals in the spin exchange interactions.

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