Abstract Submitted
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Ab initio study of the anti-ferromagnetic, non-collinear CuB_2O_4 crystal[1] YIING-REI CHEN, Physics Department, National Taiwan Normal University, Taipei, Taiwan 116, P.-R. LEE, J.-Y. LIN, Institute of Physics, National Chiao Tung University, Hsinchu, Taiwan 300, J.-M. CHEN, National Synchrotron Radiation Research Center (NSRRC), Hsinchu, Taiwan 300, A.N. VASILIEV, Department of Low temperature Physics, Moscow State University, Moscow 119992, Russia — The spiky features in the crystal absorption spectrum, and the distinct differences in the directional oxygen K-edge absorption spectroscopy of the non-collinear anti-ferromagnetic, incommensurate CuB_2O_4, had led us to this LDA+U study of the crystal, although in the commensurate phase, due to the instrumental limitation. The calculated band structure matches the spiky features in the absorption spectrum, while the orbital analyzed DOS data explain the differences in the directional oxygen K-edge absorption spectroscopy. The two groups of dispersion-less bands, immediately above the gap, come from different groups of plaquettes, of Cu(A) and Cu(B), and are responsible for the spiky features observed experimentally.

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