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Unveiling the Origin of the Basal-plane Antiferromagnetism in the J_{eff} =1/2 Mott Insulator Ba_2IrO_4: A Density Functional and Model Hamiltonian Study YUSHENG HOU, HONGJUN XIANG, XINGAO GONG, Fudan University, KEY LABORATORY OF COMPUTATIONAL PHYSICAL SCIENCES (MINISTRY OF EDUCATION) COLLABORATION — Based on the density functional theory and our new model Hamiltonian, we have studied the basal-plane antiferromagnetism in the novel J_{eff} =1/2 Mott insulator Ba_2IrO_4. By comparing the magnetic properties of the bulk Ba_2IrO_4 with those of the single-layer Ba_2IrO_4, we demonstrate unambiguously that the basal-plane antiferromagnetism is caused by the intralyer magnetic interactions rather than by the previously proposed interlayer ones. In order to reveal the origin of the basal-plane antiferromagnetism, we propose a new model Hamiltonian by adding the single ion anisotropy and pseudo-quadrupole interactions into the general bilinear pseudo-spin Hamiltonian. The obtained magnetic interaction parameters indicate that the single ion anisotropy and pseudo-quadrupole interactions are unexpectedly strong. Systematical Monte Carlo simulations demonstrate that the basal-plane antiferromagnetism is caused by the isotropic Heisenberg, bond-dependent Kitaev and pseudo-quadrupole interactions. Our results show for the first time that the single ion anisotropy and pseudo-quadrupole interaction can play significant roles in establishing the exotic magnetism in the J_{eff} =1/2 Mott insulator.

Yusheng Hou
Fudan University

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