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Magnetic ordering in Sr_2IrO_4 from first principles SABINA RUIZ-CHAVARRIA, GREGORIO RUIZ-CHAVARRIA, PABLO DE LA MORA, Facultad de Ciencias, UNAM, CARLOS COSIO-CASTANEDA, GUSTAVO TAVIZON, Facultad de Quimica, UNAM — Sr_2IrO_4 is a layered compound with IrO_2 planes, separated by two SrO planes. Experimentally Sr_2IrO_4 shows weak ferromagnetism. This behavior can be assigned either as band magnetism or canted antiferromagnetic ordering. The latter has been confirmed by Arpes. With DFT calculations (using the WIEN2k package and Quantum Expresso) we show that the antiferromagnetic ordering is more stable than the ferromagnetic one, and due to the Dzyaloshinskii-Moriya rules there is a possibility of canted magnetic ordering.

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