Magnetic ordering in $\text{Sr}_2\text{IrO}_4$ from first principles

SABINA RUIZ-CHAVARRIA, GREGORIO RUIZ-CHAVARRIA, PABLO DE LA MORA, Facultad de Ciencias, UNAM, CARLOS COSIO-CASTANEDA, GUSTAVO TAVIZON, Facultad de Química, UNAM — Sr$_2$IrO$_4$ is a layered compound with IrO$_2$ planes, separated by two SrO planes. Experimentally Sr$_2$IrO$_4$ 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.