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Magnetic properties of Sr_2IrO_4 a DFT stud PABLO DE LA MORA, Fac. de Ciencias, CARLOS COSIO-CASTANEDA, GUSTAVO TAVIZON, Fac. de Quimica, Universidad Nacional Autonoma de Mexico — Sr_2IrO_4 is a magnetic insulator with a small Ir-magnetic moment [1]. IrO_4 rotations (due to the $I41/acd$ space group) allow non-collinear magnetic ordering, thus this material could have weak ferromagnetism (non-collinear antiferromagnetically ordered Ir magnetic moments); other possible explanation is band-magnetism. Simple DFT calculations give a non-magnetic conductor. Intra-atomic electron repulsion can generate magnetic moments in the d-orbitals (via the Hubbard U (U_H)), but due to extended character of these $5d$-orbitals the U_H should be quite small. Sr_2IrO_4 is analyzed with the $WIEN2k$ package. Different magnetic configurations with varying U_H are calculated in order to try to explain the observed magnetic behaviour. [1] C Cosío-Castaneda, G Tavizón, A Baeza and R Escudero, *J. Phys.: Cond. Matter* **19** (2007) 446210

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