Theory of magnetic structure in layered iridates: spin-orbit band or Mott insulators

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In iridates, owing to strong spin-orbit coupling, the effective total angular momentum j=1/2 band is well separated from the rest of bands. In particular Sr_2IrO_4 (Sr-214) and $Sr_3Ir_2O_7$ (Sr-327) are magnetic insulators formed in j=1/2 bands leading to an interesting proposal named spin-orbit Mott insulators. However, given that there is an even number of Ir atoms per unit cell due to a staggered rotation of octahedra and even number of layers, the non-interacting system could be a spin-orbit band insulator, questioning the Mottness in these materials. To answer the question on the nature of the insulating phases, and different phases in various layered structures, we study a Hubbard model with a tight-binding spectrum designed for each Sr-214, Sr-327 and $SrIrO_3$ (Sr-113). A canted antiferromagnet (AF) is found in Sr-214 which is deep in the insulating phase close to strong coupling limit, while a collinear AF with c-axis moments is realized in Sr-327 near the spin-orbit band insulator. In contrast, Sr-113 is semimetallic. The origin of such a disimilarity is explained, and implications of our results in relation to possible high temperature superconductors in doped iridates are further discussed.