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Spin-orbit effects in iridates via electronic structure calculations: effects of tension and dimensionality[1] VICTOR PARDO, Universidade Santiago de Compostela, JOSE L. LADO, International Iberian Nanotechnology Laboratory — Ab initio calculations have been performed in $5d^5$-electron-based oxides in the large spin-orbit coupling limit. Our work tries to analyze the effects of strain and dimensionality in the electronic structure properties of iridates with Ir^{4+}:$5d^5$ electronic configuration in order to understand the different set of properties these materials present: they can be either metals or insulators, e.g. We focus on studying how close to the fully ionic j_{eff}=1/2 limit the system is by analyzing the L_z/S_z ratio. We observe that it varies continuously as a function of strain or pressure, changing drastically with relatively small variations. We also analyze what effects on the band structure accompany this variation. In order to do this, we needed to include a full non-collinearity in the calculation of spin-orbit interaction. We have explored $SrIrO_3$, Sr_2IrO_4, $Sr_3Ir_2O_7$, thin films of $SrIrO_3$ so as to analyze the dimensionality effects and the structural implications.

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