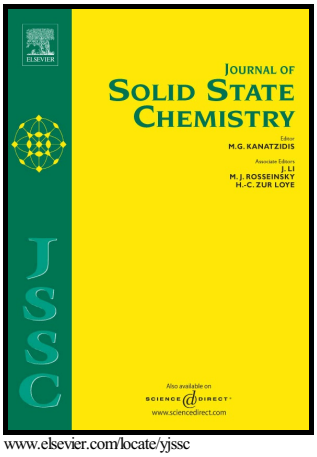

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Abstract.

Based on crystal chemistry analysis within Ca-Ir-O ternary, the generic $(CaO)_nIrO_2$ formula leading to $CaIrO_3$ for n= 1, Ca_2IrO_4 for n= 2 and Ca_4IrO_6 for n= 4 actual chemical compounds show significant structural changes regarding the spatial arrangement of IrO_6 octahedra whereby increasing amounts of CaO act as 'chemical scissor' decreasing the dimensionality of stacking octahedra from 3D (IrO_2) to 0D (Ca_4IrO_6). This is accompanied by changes in the electronic structure investigated within density functional theory. Such changes are particularly exhibited by linear increase of Ir density of states at the Fermi level revealing increasing localization of d states with crystal field effects. Eventually only for Ca_4IrO_6 a magnetic instability occurs in non magnetic configuration. Spin polarized calculations lead to development of small magnitude but finite magnetization on Ir with M ~ 0.50 μ_B totally polarized along minority spin channel ↓.

Graphical abstract

Sketches of the crystal structures highlighting the arrangement of IrO6 octahedra (green and red); a) IrO2, b) CaIrO3, c) Ca2IrO4, d) Ca4IrO6 (large grey spheres designate Ca).