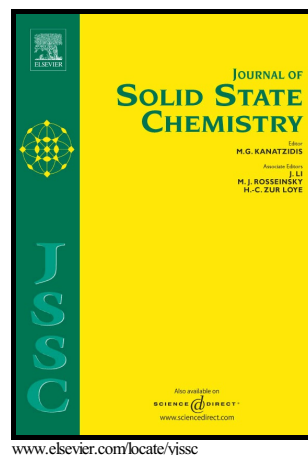


$(\text{CaO})_n\text{IrO}_2$  ( $n=1,2,4$ ) family: chemical scissors effects of CaO on structural characteristics correlated to physical properties. Ab initio study

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PII: S0022-4596(17)30237-2  
DOI: <http://dx.doi.org/10.1016/j.jssc.2017.06.016>  
Reference: YJSSC19834

To appear in: *Journal of Solid State Chemistry*

Received date: 23 March 2017

Revised date: 25 May 2017

Accepted date: 17 June 2017

Cite this article as: Samir F Matar and Jean Etourneau,  $(\text{CaO})_n\text{IrO}_2$  ( $n=1,2,4$ ) family: chemical scissors effects of CaO on structural characteristics correlated to physical properties. Ab initio study, *Journal of Solid State Chemistry*, <http://dx.doi.org/10.1016/j.jssc.2017.06.016>

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**(CaO)<sub>n</sub>IrO<sub>2</sub> (n=1,2,4) family: chemical scissors effects of CaO on structural characteristics correlated to physical properties. Ab initio study.**

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**Abstract.**

Based on crystal chemistry analysis within Ca-Ir-O ternary, the generic (CaO)<sub>n</sub>IrO<sub>2</sub> formula leading to CaIrO<sub>3</sub> for n= 1, Ca<sub>2</sub>IrO<sub>4</sub> for n= 2 and Ca<sub>4</sub>IrO<sub>6</sub> for n= 4 actual chemical compounds show significant structural changes regarding the spatial arrangement of IrO<sub>6</sub> octahedra whereby increasing amounts of CaO act as ‘chemical scissor’ decreasing the dimensionality of stacking octahedra from 3D (IrO<sub>2</sub>) to 0D (Ca<sub>4</sub>IrO<sub>6</sub>). 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<sub>4</sub>IrO<sub>6</sub> a magnetic instability occurs in non magnetic configuration. Spin polarized calculations lead to development of small magnitude but finite magnetization on Ir with  $M \sim 0.50 \mu_B$  totally polarized along minority spin channel ↓.

**Graphical abstract**

Sketches of the crystal structures highlighting the arrangement of IrO<sub>6</sub> octahedra (green and red); a) IrO<sub>2</sub>, b) CaIrO<sub>3</sub>, c) Ca<sub>2</sub>IrO<sub>4</sub>, d) Ca<sub>4</sub>IrO<sub>6</sub> (large grey spheres designate Ca).

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