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**Electronic structure and vacancy formation in La(1-x)B(x)CoO3 (B=Mg,Ca,Ba and x=0.125)** OMOTAYO SALAWU, LIYONG GAN, UDO SCHWINGENSCHLOGL, King Abdullah Univ — The $LaCoO_3$ class of materials is of interest for cathodes of solid oxide fuel cells. Spin-polarized density functional theory is applied to cubic $La_{0.75}(Mg/Ca/Ba)_{0.125}CoO_3$. The effect of this cation doping on the electronic and magnetic properties as well as oxygen vacancy formation energy is studied. Oxygen vacancies with proximity to the dopant are energetically favourable in most cases. We discuss the effect of distortions of the $CoO_6$ octahedron on the electronic structure and the formation energy of oxygen vacancies. The order of formation oxygen is found to be Mg > Ca > Ba. Cation doping incorporates holes to the Co-O network which enhances the oxygen vacancy formation.

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