

Poster Presentation

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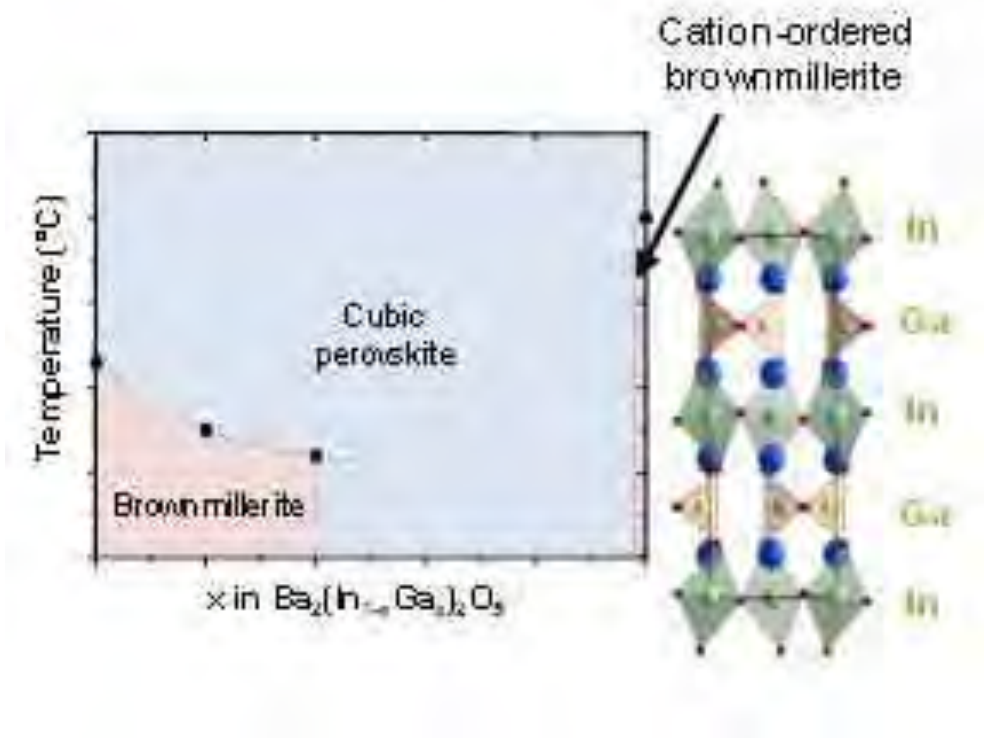
Overlooked cation-ordered brownmillerite in $Ba_2(In_{1-x}Ga_x)_2O_5$

C. Didier¹, J. Claridge¹, M. Rosseinsky¹

¹University of Liverpool, Department of Chemistry, Liverpool, United Kingdom

As Goodenough showed 20 years ago, [1] $Ba_2In_2O_5$ undergoes a transition from brownmillerite to cubic perovskite at higher temperatures, where it becomes a good oxygen ionic conductor. Past studies on doping gallium onto the indium sites [2] showed that higher Ga contents decrease the temperature required for the disordering to occur, in accordance with a higher structural disorder on the B site. In this work, we have showed that past studies on $Ba_2(In_{1-x}Ga_x)_2O_5$ have overlooked a special ordering for the Ba_2InGaO_5 composition. Combined structure refinements of neutron and X ray powder diffraction show that this material adopts a brownmillerite structure below 1200°C with a layered ordering of In and Ga. This is one of a few examples of such an ordering in the brownmillerite structure only due to size difference between the B cations. This ordering further stabilizes the brownmillerite crystal structure compared to other compositions at smaller Ga contents. As could be expected, such stronger ordering is detrimental to ionic conductivity. At 1300°C, the material disorders into a cubic perovskite structure, which was already observed in past studies. However this polymorph has an unreported red colour, which was unexpected for a material with no incompletely filled orbitals. Incorporation of oxygen interstitial defects, on the basis of conductivity versus variable oxygen experiments and spectroscopic measurements, could be at the origin of this colouration much like in TiO_2 . [3] Unfortunately photocatalytic activity for water splitting could not be tested due to the strong instability of this material towards water.

[1] J.B. Goodenough, J.E. Ruiz-Diaz, Y.S. Zhen, *Solid State Ionics*, 1990, 44, 21-31, [2] H. Yamamura, H. Hamazaki, K. Kakinuma, et al. *Journal of Korean Physical Society*, 1999, 35, [3] V. Etacheri, M. K. Seery, S. J. Hinder, et al. *Advanced Functional Materials*, 2011, 21(19), 3744–3752



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