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Successive coupled charge, magnetic, and structural transitions in $Ca_{0.5}Bi_{0.5}FeO_3$ FABIO DENIS ROMERO, YOSHITERU HOSAKA, NORIYA ICHIKAWA, TAKASHI SAITO, University of Kyoto, GRAHAM MCNALLY, J. PAUL ATTFIELD, University of Edinburgh, YUICHI SHIMAKAWA, University of Kyoto — Stoichiometric $Ca_{0.5}Bi_{0.5}FeO_3$ containing high-valent $Fe^{3.5+}$ adopting the perovskite structure was prepared under a high oxygen pressure and shows two successive phase transitions on cooling at 240 K and 200 K. Mössbauer spectroscopy and neutron powder diffraction data indicate that these transitions are associated with charge changes to relieve the instability of $Fe^{3.5+}$.The first transition is due to charge disproportionation of the iron centers while the second is due to intermetallic charge transfer between A-site Bi and B-site Fe. The transitions can be described as:
$(Ca^{2+}_{0.5}Bi^{3+}_{0.5})Fe^{3.5+}O_3 \rightarrow (Ca^{2+}_{0.5}Bi^{3+}_{0.5})(Fe^{(3.5-x)+}_{0.67}Fe^{(3.5+2x)+}_{0.33})O_3 \rightarrow$
$(Ca^{2+}_{0.5}Bi^{3+}_{0.25}Bi^{5+}_{0.25})Fe^{3+}O_3$
In the intermediate temperature phase, one third of B-sites ($Fe^{(3.5+2x)+}$) do not contribute to the magnetic scattering while the remaining spins couple antiferromagnetically. The lowest temperature magnetic structure is simple G-type antiferromagnetic resulting from a structure containing only Fe^{3+}. Competing intermetallic and disproportionation charge instabilities result in a variety of electronic, magnetic, and structural ground states.

Fabio Denis Romero
University of Kyoto

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