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A-site and B-site charge orderings of perovskite PbCoO₃ YUKI SAKAI, Kanagawa Academy of Science and Technology, RUNZE YU, HAJIME YAMAMOTO, HAJIME HOJO, MASAKI AZUMA, Tokyo Institute of Technology, IKUYA YAMADA, Osaka Prefecture University, JUNYE YANG, YUNYU YIN, YOUWEN LONG, Chinese Academy of Sciences, PING MIAO, SANGHYUN LEE, SHUKI TORII, TAKASHI KAMIYAMA, High Energy Accelerator Research Organization (KEK) — Metal ions with half-integer valence tend to split into two integer valence ions and these get spatially ordered as typically observed in $La_{0.5}Ca_{0.5}Mn^{3.5+}O_3$ [1]. Perovskite PbCoO₃ synthesized at 12 GPa was found to have an unusual average charge distribution of $Pb^{3.5+}Co^{2.5+}O_3$ with half-integer valences in both of A and B sites. Comprehensive studies using electron diffraction (ED), synchrotron X-ray diffraction (SXRD), neutron powder diffraction (NPD) and measurements of magnetic and electrical properties provide evidence of lead ion and cobalt ion charge ordering leading to $Pb^{2+}Pb_3^{4+}Co_2^{2+}Co_2^{3+}O_{12}$ quadruple perovskite structure. Here we show that half-integer valence states in both the A and B sites can be stabilized by tuning the energy levels of Pb 6s and transition metal 3d orbitals. [1] P. G. Radaelli et al., Phys. Rev. B 55, 3015–3023 (1997).

> Yuki Sakai Kanagawa Academy of Science and Technology

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