Electronic Supporting Information for:

High pressure synthesis of quasi-one-dimensional $GdFeO_3$-type perovskite $PrCuO_3$ with nearly divalent Cu ions

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1. High pressure synthesis

We have performed high pressure oxygen annealing for the oxygen deficient perovskite $PrCuO_{2.5}$ at several temperatures 420-500 °C under a high pressure of 7.5 GPa. Since $NaClO_3$ does not release oxygen below 420 °C and the impurity phase of PrO_2 appears above 450 °C, we concluded that the optimum annealing temperature is about 440 °C at a high pressure of 7.5 GPa. Furthermore, we have confirmed that the oxidizer $NaClO_3$ should be mixed with the oxygen deficient perovskite $PrCuO_{2.5}$ to obtain the fully oxidized $PrCuO_3$.

The XRD patterns of $PrCuO_{2.5}$ and $PrCuO_3$, which was obtained by the high-pressure oxygen annealing for $PrCuO_{2.5}$ at 450 °C and 7.5 GPa, are shown in Fig. S1. All the peaks for $PrCuO_{2.5}$ can be indexed with an orthorhombic unit cell (*Pbam*) with a = 5.584 Å, b = 10.353 Å, c = 3.828 Å. The main peaks for $PrCuO_3$ can be indexed with an orthorhombic unit cell (*Pbnm*) with a = 5.301 Å, b = 6.245 Å, c = 7.278 Å. The 020 reflection with asterisk is superimposed by the main reflection from the impurity phase of PrO_2, which is absent in the sample obtained at 440 °C and 7.5 GPa.

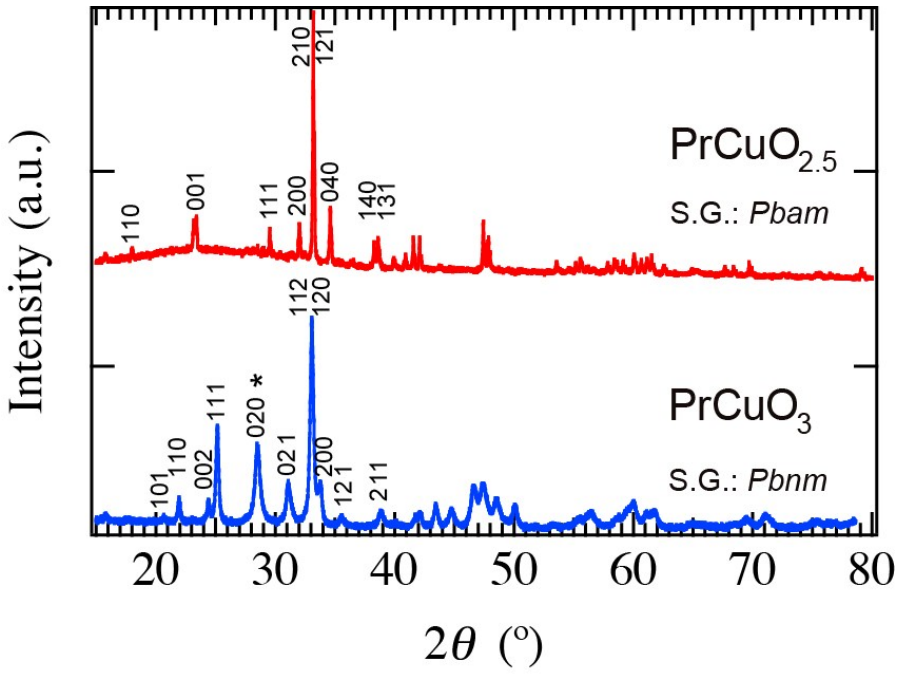

Fig. S1: XRD patterns for $PrCuO_{2.5}$ and $PrCuO_3$ measured by a Cu Kα radiation.

2. Linear interpolation analyses for XANES spectra

As shown in Fig. 4, the pre-edge structure below 8995 eV, which corresponds to the quadruple transition, is prominent especially for CuO. In order to minimize the effect of the pre-edge structure on the estimation of the absorption edge energy, we chose the intersection of the horizontal line for the linear interpolation analyses as shown in the inset of Fig. 4 (the horizontal line is located at 70% of the maximum value). On the basis of the energies of intersections for CuO and $LaCuO_3$, we define that the absorption edge energies for Cu^{2+} and Cu^{3+} states are 8996.5 eV and 8997.6 eV, respectively. Provided that the oxidation state of Cu is linearly proportional to the absorption edge energy (the linear interpolation analysis),[25] the oxidation state of Cu in $PrCuO_3$ is calculated to be +2.2.