Supporting Information

X-Ray Absorption Spectroscopic Study of the Transition-Metal-Only Double Perovskite Oxide Mn_2CoReO_6

Xiao Wang,[1,*] Jie Zhang,[1,2] Zhao Pan,[1] Dabiao Lu,[1,2] Maocai Pi,[1,2] Xubin Ye,[1] Cheng Dong,[1] Jie Chen,[3] Kai Chen,[4] Florin Radu,[5] Sonia Francoual,[6] Stefano Agrestini,[7] Zhiwei Hu,[8] Chun-Fu Chang,[8] Arata Tanaka,[9] Kazunari Yamaura,[10,11] Yao Shen,[1,2,**] and Youwen Long[1,2,12,***]

[1]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

[2]School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China

[3]Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology, Yokohama, Kanagawa 226–8503, Japan

[4]National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei 230026, China

[5]Helmholtz-Zentrum Berlin fur Materialien und Energie, Albert-Einstein-Str.15, 12489 Berlin, Germany

[6]Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany

[7]Diamond Light Source, Didcot, United Kingdom

[8]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany

[9]Quantum Matter Program, Graduate School of Advanced Science and Engineering, Hiroshima University, Higashi-hiroshima 739-8530, Japan.

[10]Research Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science, Namiki 1-1, Tsukuba, Ibaraki, 305-0044, Japan

[11]Graduate School of Chemical Sciences and Engineering, Hokkaido University, North 10 West 8, Kita-ku, Sapporo, Hokkaido, 060-0810, Japan

[12]Songshan Lake Materials Laboratory, Dongguan, Guangdong 523808, China

[*]wangxiao@iphy.ac.cn

[**]yshen@iphy.ac.cn

[***]ywlong@iphy.ac.cn

Table S1. Rietveld refinement results of MCRO. Space group is $P2_1/n$ (No. 14) with lattice parameters a = 5.23506(1) Å, b = 5.35179(1) Å, c = 7.63109(2) Å, and β = 89.966(0)°. R_{wp} = 8.21%, R_p = 4.91%, and χ^2 = 18.15.

Atom	x	y	z	Site occupancy	U_{iso} × 100 (Å^2)
Mn (4*e*)	0.4970(2)	0.5495(2)	0.7448(2)	1	0.84(3)
Co (2*c*)	0	0.5	0	0.978(2)	0.04(7)
Re (2*d*)	0.5	0	0	0.978(2)	0.16(1)
Co (2*d*) (anti-site)	0.5	0	0	0.022(2)	0.04(7)
Re (2*c*) (anti-site)	0	0.5	0	0.022(2)	0.16(1)
O(1) (4*e*)	0.3429(14)	0.2971(14)	0.9354(11)	1	0.99(2)
O(2) (4*e*)	0.3147(13)	0.3238(14)	0.5617(10)	1	0.17(2)
O(3) (4*e*)	0.8769(12)	0.4304(12)	0.7356(10)	1	0.20(2)

Table S2. Bond lengths of MCRO from the refinement. The BVS values (V_i) were calculated using the formula $V_i = \sum_j S_{ij}$, and $S_{ij} = exp[(r_0 - r_{ij})/0.37]$ with r_0 = 1.790 Å and 1.692 Å for Mn and Co, respectively.

Mn-O(1) (Å)	2.142(8), 2.611(7), 2.708(8)
Mn-O(2) (Å)	2.080(8), 2.627(8), 2.644(7)
Mn-O(3) (Å)	2.090(6). 2.148(7)
BVS (Mn)	**2.06**
Co-O(1) (Å) (×2)	2.155(8)
Co-O(2) (Å) (×2)	2.041(7)
Co-O(3) (Å) (×2)	2.151(7)
BVS (Co)	**1.93**
Re-O(1) (Å) (×2)	1.857(8)
Re -O(2) (Å) (×2)	1.956(7)
Re -O(3) (Å) (×2)	1.946(7)

Table S3. Bond angles of MCRO from the refinement.

∠Mn-O1-Co (°)	98.68(31)
∠Mn-O2-Co (°)	115.48(34)
∠Mn-O3-Co (°)	90.39(26)
∠Mn-O1-Re (°)	123.6(4)
∠Mn-O2-Re (°)	105.57(33)
∠Mn-O3-Re (°)	106.71(31)
∠Co-O1-Re (°)	137.7(4)
∠Co-O2-Re (°)	138.9(4)
∠Co-O3-Re (°)	137.25(33)