Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Two types of B-site ordered structures of the double perovskite Y_2CrMnO_6: experimental identification and first-principles study

Weipeng Wang[1,2], Fuyang Liu[3], Xuejing Zhang[1,2], Xi Shen[1], Yuan Yao[1],

Yanguo Wang[1], Banggui Liu[1,2], Xiaoyang Liu[3*], Richeng Yu[1,2*]

1. Beijing National Laboratory of Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, P. R. China.

2. School of Physical Sciences, University of Chinese Academy of Sciences

3. State key laboratory of inorganic synthesis and preparative chemistry, Jilin University, Changchun 130012, P. R. China.

* Corresponding authors: rcyu@aphy.iphy.ac.cn; liuxy@jlu.edu.cn.

(1) The proposed structure model corresponding to the rock-salt ordered structure:

Crystal system: Monoclinic

Space group: *Pc*

Cell length a	7.7756
Cell length b	6.0427
Cell length c	9.6453
Cell angle alpha	90.0000
Cell angle beta	144.2404
Cell angle gamma	90.0000

	Atom	Site			Occupancy
1	Cr	0.99956	0.74566	0.00029	1.00
2	Mn	0.49864	0.74972	0.00011	1.00
3	O	0.24274	0.06969	0.79458	1.00
4	O	0.76005	0.44156	0.20651	1.00
5	O	0.86352	0.03953	0.81078	1.00
6	O	0.13302	0.55226	0.68692	1.00
7	O	0.64439	0.21644	0.39219	1.00
8	O	0.35673	0.29287	0.61043	1.00
9	O	0.76502	0.82674	0.51870	1.00
10	O	0.22794	0.67722	0.47950	1.00

(2) The proposed structure model corresponding to the layer ordered structure:

Crystal system: monoclinic

Space group: *Pc*

Cell length a	8.2194
Cell length b	5.5349
Cell length c	5.8256
Cell angle alpha	90.0000
Cell angle beta	89.8304
Cell angle gamma	90.0000

	Atom	Site			Occupancy
1	Cr	0.00130	0.24982	0.00015	1.00
2	Mn	0.50179	0.25049	0.99981	1.00
3	O	0.06708	0.55050	0.21086	1.00
4	O	0.93439	0.05038	0.28870	1.00
5	O	0.54519	0.94450	0.80211	1.00
6	O	0.45654	0.44446	0.69832	1.00
7	O	0.76976	0.64297	0.46306	1.00
8	O	0.23329	0.14249	0.03745	1.00
9	Y	0.74502	0.22388	0.56512	1.00
10	Y	0.25784	0.72406	0.93442	1.00