## Journal of Materials Chemistry A



## CORRECTION

View Article Online



Cite this: J. Mater. Chem. A, 2018, 6,

## Correction: First-principles computational studies on layered Na<sub>2</sub>Mn<sub>3</sub>O<sub>7</sub> as a high-rate cathode material for sodium ion batteries

Zihe Zhang,<sup>a</sup> Dihua Wu,<sup>a</sup> Xu Zhang,<sup>a</sup> Xudong Zhao,<sup>a</sup> Haichang Zhang,<sup>b</sup> Fei Ding,<sup>b</sup> Zhaojun Xie<sup>a</sup> and Zhen Zhou\*<sup>a</sup>

DOI: 10.1039/c8ta90051e

www.rsc.org/MaterialsA

Correction for 'First-principles computational studies on layered Na<sub>2</sub>Mn<sub>3</sub>O<sub>7</sub> as a high-rate cathode material for sodium ion batteries' by Zihe Zhang et al., J. Mater. Chem. A, 2017, 5, 12752-12756.

The authors regret an error in the computation of the energy of each Na atom in the Na crystal in the original manuscript. The erroneous Na reference energy led to mistaken Na adsorption energy and then the average voltage. After revision, the voltage window is changed to 5.1-4.2 V, and the last step of Na deintercalation is endothermic. Therefore, in the abstract "3.6-3.1 V" should be changed to "5.1-4.2 V". In Line 9, Left Column, Page 3, "exothermic" should be changed to "endothermic"; in Line 18, "3.60 V to 3.06 V" should be changed to "5.1 V to 4.2 V". In Line 2, Right Column, Page 4, "3.6-3.1 V" should be changed to "5.1-4.2 V". The correct version of Fig. 3 is shown below. Values in Tables S1 and S2 have also changed, and this is reflected in the updated ESI.

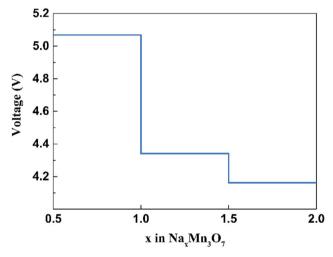


Fig. 3 The average voltage profile for Na<sub>2</sub>Mn<sub>3</sub>O<sub>7</sub> within the reversible range of 0.5–2.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

<sup>&</sup>quot;School of Materials Science and Engineering, National Institute for Advanced Materials, Computational Centre for Molecular Science, Institute of New Energy Material Chemistry, Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), Nankai University, Tianjin 300350, P. R. China. E-mail: zhouzhen@nankai.edu. cn; Fax: +86 22 23498941; Tel: +86 22 23503623

bNational Key Laboratory of Science and Technology on Power Sources, Tianjin Institute of Power Sources, Tianjin 300384, P. R. China