

UC Berkeley

UC Berkeley Previously Published Works

Title

Corrigendum: First-principles study of the nano-scaling effect on the electrochemical behavior in LiNi_{0.5}Mn_{1.5}O₄ (2013 Nanotechnology?24?424007)

Permalink

<https://escholarship.org/uc/item/65r7c32r>

Journal

Nanotechnology, 25(15)

ISSN

0957-4484

Authors

Lee, Eunseok
Persson, Kristin A

Publication Date

2014-04-01

DOI

10.1088/0957-4484/25/15/159501

Peer reviewed

CORRIGENDUM

Corrigendum: First-principles study of the nano-scaling effect on the electrochemical behavior in $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ (2013 *Nanotechnology* **24** 424007)

To cite this article: Eunseok Lee and Kristin A Persson 2014 *Nanotechnology* **25** 159501

View the [article online](#) for updates and enhancements.

Recent citations

- [Theoretical Insights into Oxidation States of Transition Metals at \(001\) and \(111\) \$\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4\$ Spinel Surfaces](#)
Nadia N. Intan *et al*

- [Density functional theory analysis of surface structures of spinel \$\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4\$ cathode materials](#)
Jianjian Shi *et al*

- [Surface stability of spinel \$\text{MgNi}_{0.5}\text{Mn}_{1.5}\text{O}_4\$ and \$\text{MgMn}_2\text{O}_4\$ as cathode materials for magnesium ion batteries](#)
Wei Jin *et al*



IOP | ebooksTM

Bringing you innovative digital publishing with leading voices to create your essential collection of books in STEM research.

Start exploring the collection - download the first chapter of every title for free.

Corrigendum: First-principles study of the nano-scaling effect on the electrochemical behavior in $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ (2013 *Nanotechnology* 24 424007)

Eunseok Lee and Kristin A Persson

Environmental Energy Technologies Division, Lawrence Berkeley National Laboratory, CA 94720, USA

E-mail: eunseoklee@lbl.gov

Received 4 March 2014

Accepted for publication 4 March 2014

Published 20 March 2014

We have found that the surface energy values in table 1 omitted a factor of 2 (see equation (1)). The correct version of table 1 is presented here. This correction does not alter the

subsequent discussions and conclusions, as all structures and facets lacked the factor of 2, and were compared relative to each other.

Table 1. Surface energy for the low index facets, (100), (110), (111), in the uniformly disordered structure, ordered structure, and ordered structure with a local inverse spinel cation ordering near the surface. Whenever a facet exhibits the same elements for different termination layers, we distinguish the slab cells by surface composition. In the uniformly disordered structure, the (110) surface composition Li:Mn:Ni is 1:2:1 and 1:1.5:0.5 in Li/Ni/Mn/O-I and -II, respectively. In the ordered structure, the (110) surface compositions are 1:2:0.25, 1:2.5:0.5, and 1:2:1 in Li/Ni/Mn/O-I, -II, and -III, respectively.

Ordering	Facet	Termination	γ (J m^{-2})
Uniform	(100)	Li/Mn/Ni/O	1.07
		Mn/Ni/O	1.73
		Mn/O	1.66
	(110)	Li/Mn/Ni/O-I	2.34
		Li/Mn/Ni/O-II	1.55
	(111)	Li/Ni/O	0.87
		Li/Mn/O	2.06
		Mn/O	1.41
		Li/Mn/Ni/O	1.11
		Mn/Ni/O	1.43
		Li/Mn/Ni/O-I	1.50
Ordered	(100)	Li/Mn/Ni/O-II	1.71
		Li/Mn/Ni/O-III	1.58
		Li/Mn/Ni/O	1.33
		Mn/Ni/O	2.04
		Li/Mn/Ni/O	1.59
	(110)	Li/Mn/Ni/O	1.82
		Li/O	1.09
		Li/Mn/O	1.23
	(111)	Li/Mn/Ni/O	1.59
		Li/O	1.82
		Li/Mn/O	1.23