Lawrence Berkeley National Laboratory
Recent Work

Title
Erratum: Computational and experimental investigation of TmAgTe2 and: XYZ 2 compounds, a new group of thermoelectric materials identified by first-principles high-throughput screening (Journal of Materials Chemistry C (2015) 3 (10554-10565))

Permalink
https://escholarship.org/uc/item/26m4g6rf

Journal
Journal of Materials Chemistry C, 4(19)

ISSN
2050-7534

Authors
Zhu, H
Hautier, G
Aydemir, U
et al.

Publication Date
2016

DOI
10.1039/c6tc90077a

Peer reviewed
Correction: Computational and experimental investigation of TmAgTe₂ and XYZ₂ compounds, a new group of thermoelectric materials identified by first-principles high-throughput screening

Hong Zhu,a Geoffroy Hautier,b Umut Aydemir,c Zachary M. Gibbs,d Guodong Li,c Saurabh Bajaj,c Jan-Hendrik Pöhls,e Danny Broberg,f Wei Chen,g Anubhav Jain,g Mary Anne White,e Mark Asta,f G. Jeffrey Snyder,c Kristin Perssonfg and Gerbrand Ceder*afg

Correction for ‘Computational and experimental investigation of TmAgTe₂ and XYZ₂ compounds, a new group of thermoelectric materials identified by first-principles high-throughput screening’ by Hong Zhu et al., J. Mater. Chem. C, 2015, 3, 10554–10565.

Some of the author affiliations are incorrect in this article. The correct details are those given in this correction and involve changes for Anubhav Jain, Mary Anne White, Mark Asta, and Kristin Persson.

On page 10562, the authors also note eqn (1) should be corrected to “$k_{\text{min}} = 0.4k_B n^2 (\nu_L + 2\nu_T)$”. The original text after eqn (1), “where $k_B$ is Planck’s constant, $\rho$ is atomic density of the materials. $\nu_L$ and $\nu_T$ can be determined from elastic constants such as bulk modulus ($K$) and shear modulus ($G$), predicted from calculations”, should appear as “where $k_B$ is Planck’s constant, $n$ is number density of atoms. $\nu_L$ and $\nu_T$ can be determined from mass density ($\rho$) and elastic constants such as bulk modulus ($K$) and shear modulus ($G$), predicted from calculations.”

On page 10557, for consistency of symbols on mass density, the original wording “$C_1 = \nu_L^2 d$ (where $\nu_L$ is the longitudinal speed of sound and $d$ is density)” should appear as “$C_1 = \nu_L^2 \rho$ (where $\nu_L$ is the longitudinal speed of sound and $\rho$ is mass density)”.

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

DOI: 10.1039/c6tc90077a

www.rsc.org/MaterialsC