



Cite this: *J. Mater. Chem. C*, 2016, **4**, 4331

## Correction: Computational and experimental investigation of $\text{TmAgTe}_2$ and $\text{XYZ}_2$ compounds, a new group of thermoelectric materials identified by first-principles high-throughput screening

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

DOI: 10.1039/c6tc90077a

[www.rsc.org/MaterialsC](http://www.rsc.org/MaterialsC)

Correction for 'Computational and experimental investigation of  $\text{TmAgTe}_2$  and  $\text{XYZ}_2$  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 " $\kappa_{\min} = 0.4k_B n^{\frac{2}{3}} (\nu_{L,s} + 2\nu_{T,s})$ ". The original text after eqn (1), "where  $k_B$  is Planck's constant,  $\rho$  is atomic density of the materials.  $\nu_{L,s}$  and  $\nu_{T,s}$  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.  $\nu_{L,s}$  and  $\nu_{T,s}$  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 " $C_1 = \nu_{L,s}^2 \rho$  (where  $\nu_{L,s}$  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.

<sup>a</sup> Department of Materials Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, Massachusetts, 02139, USA.  
E-mail: [gceder@mit.edu](mailto:gceder@mit.edu)

<sup>b</sup> Institute of Condensed Matter and Nanosciences (IMCN), Université catholique de Louvain, Chemin des étoiles 8, bte L7.03.01, Louvain-la-Neuve 1348, Belgium

<sup>c</sup> Materials Science, California Institute of Technology, 1200 E California Blvd, Pasadena, California, 91125, USA

<sup>d</sup> Division of Chemistry and Chemical Engineering, California Institute of Technology, 1200 E California Blvd, Pasadena, California, 91125, USA

<sup>e</sup> Department of Physics and Atmospheric Science, Dalhousie University, 6310 Coburg Rd., PO BOX 15000, Halifax, Nova Scotia B3H 4R2, Canada

<sup>f</sup> Department of Materials Science and Engineering, University of California, Berkeley, Berkeley, California 94720, USA

<sup>g</sup> Lawrence Berkeley National Lab, 1 Cyclotron Rd., Berkeley, California 94720, USA

