Electronic Supplementary Material (ESI) for Journal of Materials Chemistry

Supplement to

Ion transport and phase transition in $Li_{7-x}La_3(Zr_{2-x}M_x)O_{12}$ ($M = Ta^{5+}$, Nb^{5+}, $x = 0, 0.25$)

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Forcefield Parameters for MD simulations

MD simulations have been conducted with a dedicated force-field based on Morse-type interactions derived from our softBV bond valence (BV) parameters using the following forcefield library file and the software package GULP as implemented in Materials Studio 5.0:

```
#
#  Library of BV-based potential for modelling llz(t)
#
# Turn off Ewald sum and charged interactions
keyword noelectrostatics

species
Li core   0.79582
La core   1.68819
Zr core   2.25091
Ta core   2.81364
O  core  -1.25657

morse                          ener
Li core O  core      0.988160      1.937985      1.940013  0.000 0.000 10.000
La core O  core      1.185874      2.217295      2.469886  0.000 0.000 10.000
Zr core O  core      2.191032      2.040816      1.996024  0.000 0.000 10.000
Ta core O  core      2.366685      2.057613      1.855320  0.000 0.000 10.000

qerfc                          ener
Li core Li core       1.89426     10.000000
Li core La core       2.25576     10.000000
Li core Zr core       1.96656     10.000000
Li core Ta core       1.89426     10.000000
La core La core       2.61726     10.000000
La core Zr core       2.32806     10.000000
La core Ta core       2.25576     10.000000
Zr core Zr core       2.03886     10.000000
Zr core Ta core       1.96656     10.000000
Ta core Ta core       1.89426     10.000000
O  core O  core       1.92318     10.000000
```