Electronic Supplementary Material (ESI) for Journal of Materials Chemistry

Supplementary information to

Structural requirements for fast Lithium ion migration in $Li_{10}GeP_2S_{12}$

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Forcefield used in GULP for the reported MD simulations

```
#
#  Library of BV potential for modelling LGPS
#
keyword noelectrostatics molecule angle fix_molecule molq

species
Li core    0.882995
Ge core  1.765911
P  core    2.548873
S  core   -1.307770

morse                          ener
Li core S  core     1.066825     1.531394     2.349741  0.000 0.000 11.000
Ge core S  core    2.087340     1.945525     2.104578  0.000 0.000 11.000
P  core S  core     3.939695     1.766784     1.951558  0.000 0.000 10.000

qerfc                    ener
# fractional radius =  .78
Li core Li core        2.0436     11.000000
Li core Ge core       1.9656     11.000000
Li core P  core        1.8798     11.000000
Ge core Ge core    1.8876     11.000000
Ge core P  core      1.8018     11.000000
P  core P  core        1.7160     11.000000
S  core S  core        2.9562     11.000000

three cosine bond
Ge core S  core S  core 19.9999 109.471
P  core S  core S  core  19.9999 109.471
```