

Theoretical Predictions of Alkali Hexazirconate ($A_2Zr_6O_{13}$, $A = Li, Na, \text{ And } K$) as Candidates for Alkali Ion Batteries

JR. Fernández-Gamboa^{a,b}, Frederik Tielens^b, and Yohandys A. Zulueta^{a,*}

^a*Departamento de Física, Facultad de Ciencias Naturales y Exactas, Universidad de Oriente, CP- 90500, Santiago de Cuba, Cuba.*

^b*General Chemistry (ALGC) – Materials Modelling Group, Vrije Universiteit Brussel, Pleinlaan 2, 1050, Brussels, Belgium.*

*Corresponding author e-mail: jrfernandez@uo.edu.cu

Electronic Supplementary Information

The supplementary information along this manuscript contains the potential parameters (force field) used in this study, including an input file for geometry optimization of $Li_2Zr_6O_{13}$ structure, for reproducibility providing further simulation details for the readers.

Potential parameters (library.lib)

```
#####  
species  
Li core 1.0  
Na core 1.0  
K core 1.0  
O core 0.75823  
O shel -2.75823  
Si core 4.0  
Zr core 4.0  
Sn core 4.0  
Ti core 4.0  
Ni core 3.0  
Sc core 3.0  
Co core 3.0  
Fe core 3.0  
Mn core 3.0  
  
buck  
Li core O shel 632.1018 0.2906 0.0 0.0 10.0  
Na core O shel 1271.504 0.3000 0.0 0.0 10.0  
K core O shel 3587.570 0.3000 0.0 0.0 10.0
```

Si core O shel 1283.91 0.314919 10.66 0.0 10.0
Ti core O shel 5111.7 0.2625 0.0 0.0 10.0
O shel O shel 22764.30 0.149 27.62 0.0 10.0 #lewis and catlow lib
Zr core O shel 1453.8 0.35000 0.0 0.0 10.0 #lewis
Sn core O shel 1414.32 0.3479 13.66 0.0 10.0 #Grimes 2000
#trivalent
buck
Sc core O shel 1575.85 0.3211 0.0 0.0 10.0 #L. Minervini, M.O. Zacate, R.W. Grimes,
Solid State Ionics 116 (1999) 339.
Ni core O shel 1018.36 0.3299 0.0 0.0 10.0
Co core O shel 1329.82 0.3087 0.0 0.0 10.0 #Cherry, M.; Islam, M.S.; Catlow, C.R.A.
Oxygen Ion Migration in Perovskite-Type Oxides. J. Solid State Chem. 1995, 118, 125–132.
Fe core O shel 1156.36 0.3299 0.0 0.0 10.0
Mn core O shel 1257.9 0.3214 0.0 0.0 10.0

thre

Si core O core O core 2.09724 109.47 1.9 1.9 3.5

spring

O core 30.21

Input file for geometry optimization of $\text{Li}_2\text{Zr}_6\text{O}_{13}$ structure in P1 space group

opti conp conse qok nomod pres prop pot
pressure 0 GPa
ftol 1e-005
gtol 0.0001
xtol 1e-005
maxcyc 1000

title

GULP calculation from Materials Studio for $\text{Li}_2\text{Zr}_6\text{O}_{13}$

end

cell

16.517500 3.892400 9.815500 90.000000 97.726300 90.000000 1 1 1 1 1 1

fractional

Li1 core 0.458335 0.500000 0.254017 1.000000 1.000000 0.0 1 1 1
Li1 core 0.958335 0.000000 0.254017 1.000000 1.000000 0.0 1 1 1
Li1 core 0.541665 0.500000 0.745983 1.000000 1.000000 0.0 1 1 1
Li1 core 0.041665 0.000000 0.745983 1.000000 1.000000 0.0 1 1 1
Zr1 core 0.111358 0.000000 0.082668 4.000000 1.000000 0.0 1 1 1
Zr1 core 0.162623 0.000000 0.430555 4.000000 1.000000 0.0 1 1 1
Zr1 core 0.224302 0.000000 0.772487 4.000000 1.000000 0.0 1 1 1
O1 core 0.232702 0.000000 0.246312 0.758230 1.000000 0.0 1 1 1
O1 shel 0.232702 0.000000 0.246312 -2.758230 1.000000 0.0 1 1 1

O1 core 0.073477 0.000000 0.278185 0.758230 1.000000 0.0 1 1 1
O1 shel 0.073477 0.000000 0.278185 -2.758230 1.000000 0.0 1 1 1
O1 core 0.287830 0.000000 0.573742 0.758230 1.000000 0.0 1 1 1
O1 shel 0.287830 0.000000 0.573742 -2.758230 1.000000 0.0 1 1 1
O1 core 0.130647 0.000000 0.615745 0.758230 1.000000 0.0 1 1 1
O1 shel 0.130647 0.000000 0.615745 -2.758230 1.000000 0.0 1 1 1
O1 core 0.340400 0.000000 0.886590 0.758230 1.000000 0.0 1 1 1
O1 shel 0.340400 0.000000 0.886590 -2.758230 1.000000 0.0 1 1 1
O1 core 0.144922 0.000000 0.896952 0.758230 1.000000 0.0 1 1 1
O1 shel 0.144922 0.000000 0.896952 -2.758230 1.000000 0.0 1 1 1
Zr1 core 0.611358 0.500000 0.082668 4.000000 1.000000 0.0 1 1 1
Zr1 core 0.662623 0.500000 0.430555 4.000000 1.000000 0.0 1 1 1
Zr1 core 0.724302 0.500000 0.772487 4.000000 1.000000 0.0 1 1 1
O1 core 0.732703 0.500000 0.246312 0.758230 1.000000 0.0 1 1 1
O1 shel 0.732703 0.500000 0.246312 -2.758230 1.000000 0.0 1 1 1
O1 core 0.573477 0.500000 0.278185 0.758230 1.000000 0.0 1 1 1
O1 shel 0.573477 0.500000 0.278185 -2.758230 1.000000 0.0 1 1 1
O1 core 0.787830 0.500000 0.573742 0.758230 1.000000 0.0 1 1 1
O1 shel 0.787830 0.500000 0.573742 -2.758230 1.000000 0.0 1 1 1
O1 core 0.630647 0.500000 0.615745 0.758230 1.000000 0.0 1 1 1
O1 shel 0.630647 0.500000 0.615745 -2.758230 1.000000 0.0 1 1 1
O1 core 0.840400 0.500000 0.886590 0.758230 1.000000 0.0 1 1 1
O1 shel 0.840400 0.500000 0.886590 -2.758230 1.000000 0.0 1 1 1
O1 core 0.644922 0.500000 0.896952 0.758230 1.000000 0.0 1 1 1
O1 shel 0.644922 0.500000 0.896952 -2.758230 1.000000 0.0 1 1 1
Zr1 core 0.888643 0.000000 0.917332 4.000000 1.000000 0.0 1 1 1
Zr1 core 0.837377 0.000000 0.569445 4.000000 1.000000 0.0 1 1 1
Zr1 core 0.775698 0.000000 0.227513 4.000000 1.000000 0.0 1 1 1
O1 core 0.767298 0.000000 0.753688 0.758230 1.000000 0.0 1 1 1
O1 shel 0.767298 0.000000 0.753688 -2.758230 1.000000 0.0 1 1 1
O1 core 0.926523 0.000000 0.721815 0.758230 1.000000 0.0 1 1 1
O1 shel 0.926523 0.000000 0.721815 -2.758230 1.000000 0.0 1 1 1
O1 core 0.712170 0.000000 0.426258 0.758230 1.000000 0.0 1 1 1
O1 shel 0.712170 0.000000 0.426258 -2.758230 1.000000 0.0 1 1 1
O1 core 0.869353 0.000000 0.384255 0.758230 1.000000 0.0 1 1 1
O1 shel 0.869353 0.000000 0.384255 -2.758230 1.000000 0.0 1 1 1
O1 core 0.659600 0.000000 0.113410 0.758230 1.000000 0.0 1 1 1
O1 shel 0.659600 0.000000 0.113410 -2.758230 1.000000 0.0 1 1 1
O1 core 0.855078 0.000000 0.103048 0.758230 1.000000 0.0 1 1 1
O1 shel 0.855078 0.000000 0.103048 -2.758230 1.000000 0.0 1 1 1
Zr1 core 0.388643 0.500000 0.917332 4.000000 1.000000 0.0 1 1 1
Zr1 core 0.337377 0.500000 0.569445 4.000000 1.000000 0.0 1 1 1
Zr1 core 0.275698 0.500000 0.227513 4.000000 1.000000 0.0 1 1 1
O1 core 0.267297 0.500000 0.753688 0.758230 1.000000 0.0 1 1 1
O1 shel 0.267297 0.500000 0.753688 -2.758230 1.000000 0.0 1 1 1
O1 core 0.426522 0.500000 0.721815 0.758230 1.000000 0.0 1 1 1
O1 shel 0.426522 0.500000 0.721815 -2.758230 1.000000 0.0 1 1 1
O1 core 0.212170 0.500000 0.426258 0.758230 1.000000 0.0 1 1 1
O1 shel 0.212170 0.500000 0.426258 -2.758230 1.000000 0.0 1 1 1
O1 core 0.369353 0.500000 0.384255 0.758230 1.000000 0.0 1 1 1

O1 shel 0.369353 0.500000 0.384255 -2.758230 1.000000 0.0 1 1 1
O1 core 0.159600 0.500000 0.113410 0.758230 1.000000 0.0 1 1 1
O1 shel 0.159600 0.500000 0.113410 -2.758230 1.000000 0.0 1 1 1
O1 core 0.355078 0.500000 0.103048 0.758230 1.000000 0.0 1 1 1
O1 shel 0.355078 0.500000 0.103048 -2.758230 1.000000 0.0 1 1 1
O1 core 0.000000 0.000000 0.000000 0.758230 1.000000 0.0 1 1 1
O1 shel 0.000000 0.000000 0.000000 -2.758230 1.000000 0.0 1 1 1
O1 core 0.500000 0.500000 0.000000 0.758230 1.000000 0.0 1 1 1
O1 shel 0.500000 0.500000 0.000000 -2.758230 1.000000 0.0 1 1 1

Species

Li1 core Li

O1 core O

O1 shel O

Zr1 core Zr

spacegroup

P 1

library library.lib

dump Li2Zr6O13.grs

output movie arc Li2Zr6O13