Contribution ID: **28** Type: **Talk**

Investigating the Pressure Effects on Structural Behaviour of Garnet-Type Li7La3Zr2O12 Solid Electrolyte Material: A Classical Molecular Dynamics Study

Thursday, 2 December 2021 11:30 (30 minutes)

The cubic garnet-type Li7La3Zr2O12 is an eminent candidate for next-generation solid state battery technology due to its thermal stability and high ionic conductivity. As such, its operation mechanisms need to be thoroughly understood, particularly focusing on the structural instability challenge reported to occur at lower temperatures. Herein, the statistical sampling capability of molecular dynamics simulations is employed during the investigation of fundamental structural, kinetic and thermodynamic properties emanating its subjection to pressure and temperature. Systematic induction of pressure yielded transition of the tetragonal phase to the cubic phase at 2 GPa pressure. The lattice parameters for the cubic and tetragonal phases, acquired in the current study are within 0.38 % agreement with literature. Furthermore, the XRD graphs confirm varying phases under different pressure conditions. The temperature phase diagram for 0 GPa structure agrees well with the literature trends and interestingly, the 2 GPa structure retained the cubic phase at various temperatures and confirmed in the XRDs and temperature phase diagram. Interrogation of LaO8 dodecahedral and ZrO6 octahedra demonstrated no significant variations in bond lengths and bond angles giving a good indication for the regulation of Li+-transport channel size in the 2 GPa structure. Efforts in this study are a preliminary stage to fully understanding the thermodynamic impact as a structural modification avenue pending further investigations.

Student?

No

Supervisor name

Supervisor email

Primary author: Prof. LEDWABA, Raesibe Sylvia (University of Limpopo)

Presenter: Prof. LEDWABA, Raesibe Sylvia (University of Limpopo)

Session Classification: HPC Applications

Track Classification: Materials Science