Topological Analysis of Lithium Migration Paths: Application to Solid Electrolytes

Lincoln Miara[a], Masoud Aryanpour[a], Shyue Ping Ong[b], Yifei Mo[b], Gerbrand Ceder[b], Hyo Sug Lee[a]

[a]Samsung Advanced Institute of Technology – USA, Cambridge MA, 02142
[b]Department of Materials Science, Massachusetts Institute of Technology, Cambridge, MA 02139

All solid state rechargeable lithium batteries are considered a promising next-generation technology compared to conventional Li-ion batteries since they may have sufficiently low cost and high energy density for use in electric vehicles.

At present, however, no material can simultaneously satisfy the requirements of high ionic conductivity and negligible electronic conductivity, and a wide electrochemical stability window [1]. To investigate the role of the geometric framework on the lithium diffusivity, we have performed both a topological analysis of the crystal structure, as well as ab initio molecular dynamics (AIMD).

Figure 1 shows a comparison between AIMD results (left) from [2] and our topological analysis (right) on the recently identified superionic conductor $Li_{10}GeP_2S_{12}$ (LGPS) [3]. The positive correlations we observe validate the use of the topological analysis as a rapid methodology to analyze and gather information on the size and shape of conduction paths for different crystal structures. Furthermore, by comparing topological results and AIMD results, it is possible to correlate transport properties with geometric features, e.g., activation energy with bottleneck size. These correlations allow us to better understand the nature of conduction in solid-state lithium ion conducting materials.

The rules governing the relationship between geometric parameters and transport properties such as diffusivity and activation energy are presented.

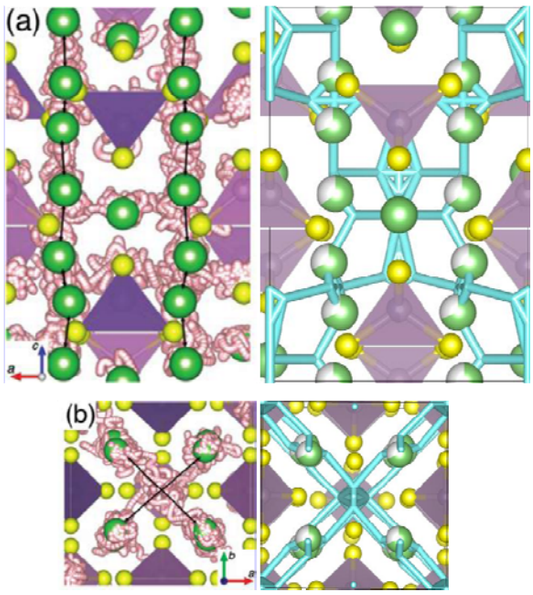

Figure 1: Comparison of results on $Li_{10}GeP_2S_{12}$ between ab initio molecular dynamics (left side) [2], and migration path analysis (right-side). The bottleneck size is 1.87 A.

REFERENCES:

1. E. Quartarone, and P. Mustarelli, *Chemical Society reviews*, 2525-40, 40, (5), 2011.
2. Y. Mo, S. P. Ong and G. Ceder, *Chem. Mater.*, 2012, 24, 15
3. N. Kamaya, et al., *Nature Materials*, 682-686, 10, (9), 2011