Fast diffusion mechanism in $Li_4P_2S_6$ via a concerted process of interstitial Li ions

Andreas R. Stamminger,^{*,†,‡} Benedikt Ziebarth,[†] Matous Mrovec,[‡] Thomas

Hammerschmidt, ‡ and Ralf Drautz ‡

†Robert Bosch GmbH, Corporate Research, 71272, Renningen, Germany
‡Ruhr-Universität Bochum, Interdisciplinary Centre for Advanced Materials Simulation,
Universitätsstraße 150, 44801, Bochum, Germany

E-mail: andreas.stamminger@de.bosch.com

Supplementary Material



Figure S1: Raw data of the $MSD^{(\text{Li})}(t)$ dependencies captured from the 300 ps AIMD runs. Although the temperatures are chosen rather high, strong non-linear features are still clearly visible from the data.



Figure S2: NEB paths for interstitial lithium migration following the path along $int3 \rightarrow int1 \rightarrow int1$. The plot shows the results for this path obtained by Dietrich et al.¹ (blue) and the NEB path calculated in this work (purple). A fit to the data points calculated in this work is indicated by the blue line. (Note that we adopted the notation chosen by Dietrich et al. to label interstitial sites to enhance comparability)



Figure S3: NEB paths for interstitial lithium migration following the path along $int3 \rightarrow int1 \rightarrow int2 \rightarrow int2$. The plot shows the results for this path obtained by Dietrich et al.¹ (blue) and the NEB path calculated in this work (purple). A fit to the data points calculated in this work is indicated by the blue line. (Note that we adopted the notation chosen by Dietrich et al. to label interstitial sites to enhance comparability)

References

 Dietrich, C.; Sadowski, M.; Sicolo, S.; Weber, D. A.; Sedlmaier, S. J.; Weldert, K. S.; Indris, S.; Albe, K.; Janek, J.; Zeier, W. G. Local Structural Investigations, Defect Formation, and Ionic Conductivity of the Lithium Ionic Conductor Li₄P₂S₆. *Chem. Mater.* , *28*, 8764–8773.