

Table 1 Li⁺ diffusion barriers based on the different diffusion paths in LLTO|Li interface.

| Li1-Li2/Å | Li ⁺ diffusion barrier/eV | Li2-Li3/Å | Li ⁺ diffusion barrier/eV |
|-----------|--------------------------------------|-----------|--------------------------------------|
| 0 | 0 | 0 | 0 |
| 1.57989 | 0.11198 | 0.69589 | 0.15424 |
| 2.97921 | 0.56293 | 2.487 | 0.60757 |
| 4.28792 | 1.08265 | 4.17352 | 1.17782 |
| 5.59101 | 1.23404 | 5.7656 | 1.25969 |
| 6.6945 | -0.09245 | 7.48079 | -0.1 |

Table 2 Li⁺ diffusion barriers based on the different diffusion paths in LLTO|LiIn₂ interface.

| Li1-Li2/Å | Li ⁺ diffusion barrier/eV | Li2-Li3/Å | Li ⁺ diffusion barrier/eV | Li3-Li4/Å | Li ⁺ diffusion barrier/eV |
|-----------|--------------------------------------|-----------|--------------------------------------|-----------|--------------------------------------|
| 0 | 0 | 0 | 0 | 0 | 0 |
| 1.02957 | 0.97477 | 0.71892 | 1.21451 | 0.90389 | 0.88539 |
| 2.00572 | 0.08921 | 1.38081 | 0.16204 | 1.8079 | 0.05249 |
| 2.9317 | 0.08069 | 2.1101 | 0.05019 | 2.67348 | 0.11214 |
| 3.82689 | 0.87719 | 2.73717 | 0.63227 | 3.70845 | 1.03035 |