

Li-ion conductivity in $\text{Li}_9\text{S}_3\text{N}$ – Supplementary Information

Lincoln Miara¹, Naoki Suzuki², William Davidson Richards³, Yan E. Wang³, Jae Chul Kim³, Gerbrand Ceder³

¹Samsung Advanced Institute of Technology – USA, 255 Main St., Suite 702, Cambridge, MA 02142

²Samsung Research Japan— Mino Semba Center Bldg. 13F, 2-1-11, Semba Nish Minoh, Osaka 562-0036,
Japan

³Department of Materials Science and Engineering, Massachusetts Institute of Technology, 77

Massachusetts Ave, Cambridge, MA 02139

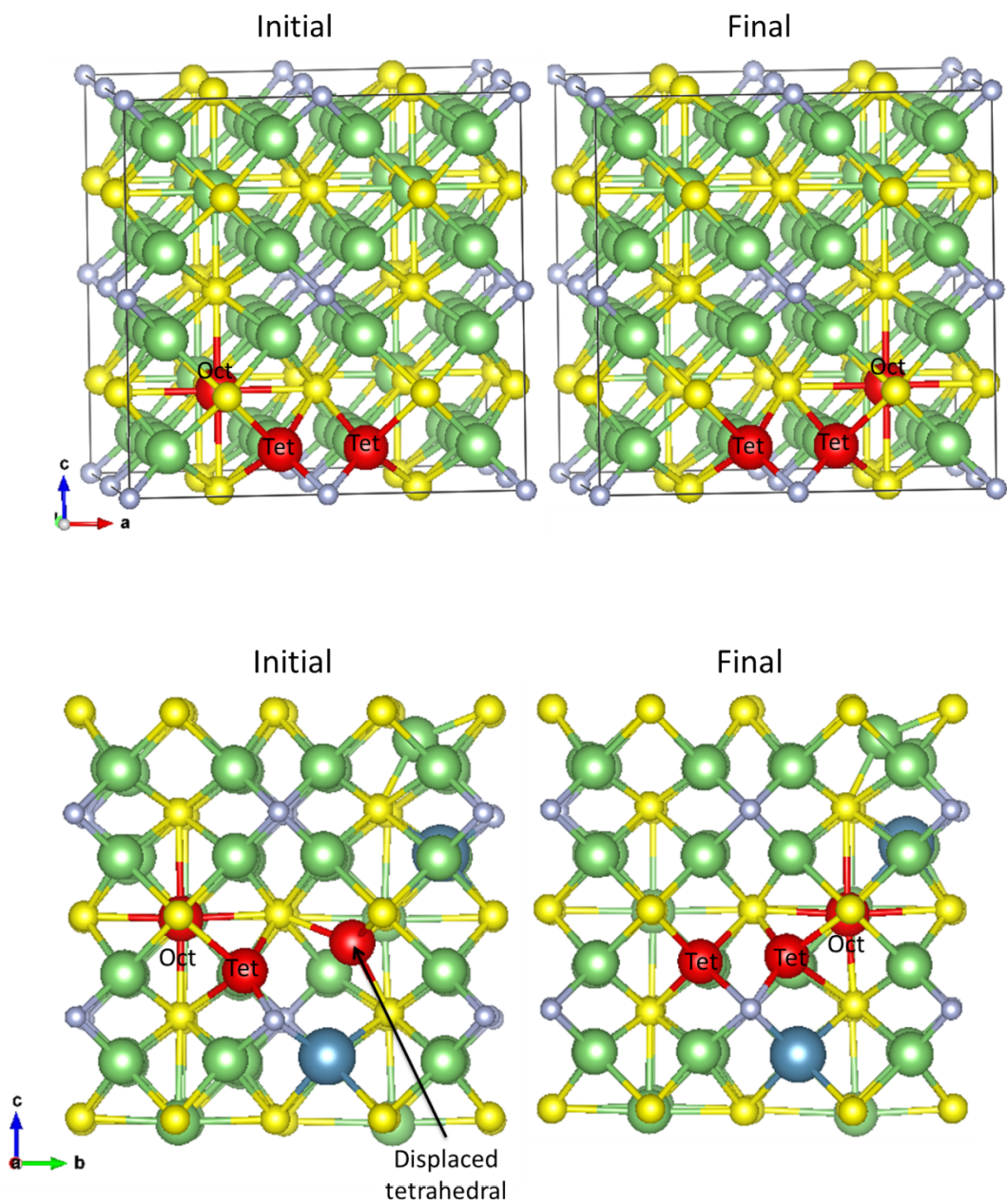


Figure S1: Initial and final images of the NEB pathways explored. (Top) LSN, the 3-Li coordinated hop mechanism is shown where the coordinated 3 hop mechanism requires 3 Li to pass through the triangular sulfur bottleneck. (Bottom) Li_{8.5}Ca_{0.25}S₃N, the initial image shows the Li displaced from the tetrahedral site near a Ca dopant along the migration pathway. Thus, only 2 Li are required to pass through the bottleneck and the migration barrier is decreased.

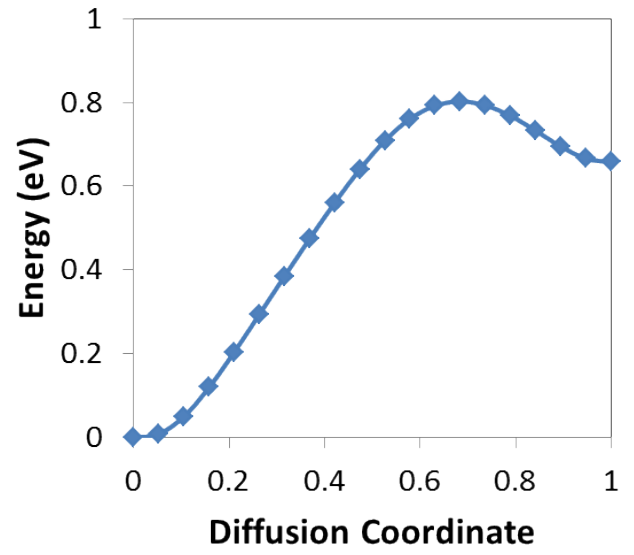
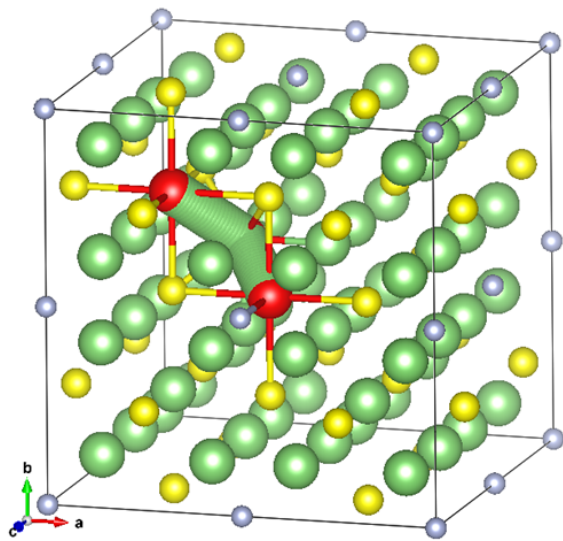


Figure S2: 2 Li atom migration pathway from 6S-coordinated octahedral site to 4S-2N-coordinated octahedral site via tetrahedral site. The migration energy is calculated to be about 0.8 eV.