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# Supplemental Information for

## First-Principles Explorations of the Electrochemical Lithiation Dynamics of a Multilayer Graphene Nanosheet-based Sulfur-Carbon Composite

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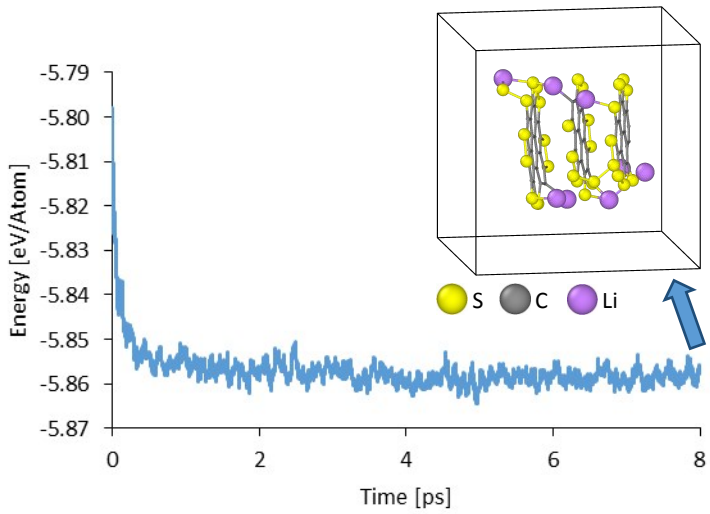


Figure S1: AIMD energy profile at a Li/S molar ratio of 0.25. DOL molecules not shown for clarity.

Table S1: The table below shows the total energy at three different lithium contents after structural optimizations (SC-Li composite + DOL) performed with and without spin polarization. Comparison between the two calculations shows no energy differences above 4x10-4 eV. With our systems having up to 544 atoms on average, this energy difference is considered negligible, leading us to ignore spin polarization effects in our calculations

| Li:S | Non Spin polarized [eV] | Spin Polarized [eV] | Spin - Non Spin polarized [eV] |
|---|---|---|---|
| 0.00:1 | -3.11E+03 | -3.11E+03 | -0.00040 |
| 1.00:1 | -3.23E+03 | -3.23E+03 | -0.00040 |
| 2.00:1 | -3.15E+03 | -3.15E+03 | -0.00040 |