Supplementary Information: Density functional theory studies on sulfur-poly(acrylonitrile) as a cathode host material for lithium-sulfur batteries

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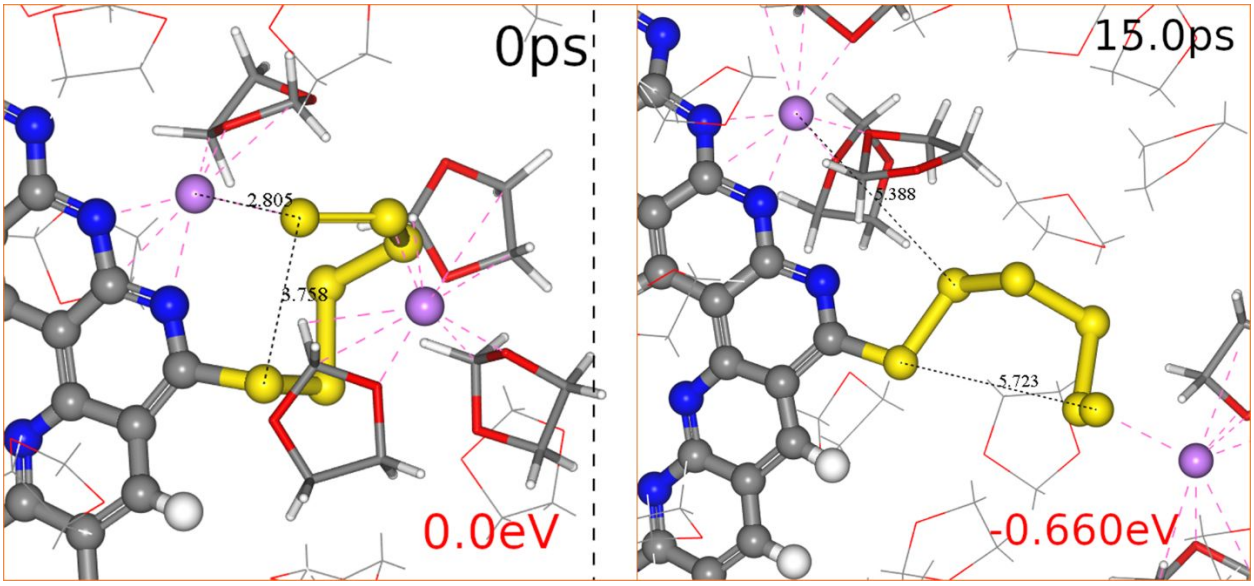

Figure S1: Evolution of the system, where initially the PS is attached to the polymer. As described in **Figure 1A**. Color coding is described in **Figure 1**.

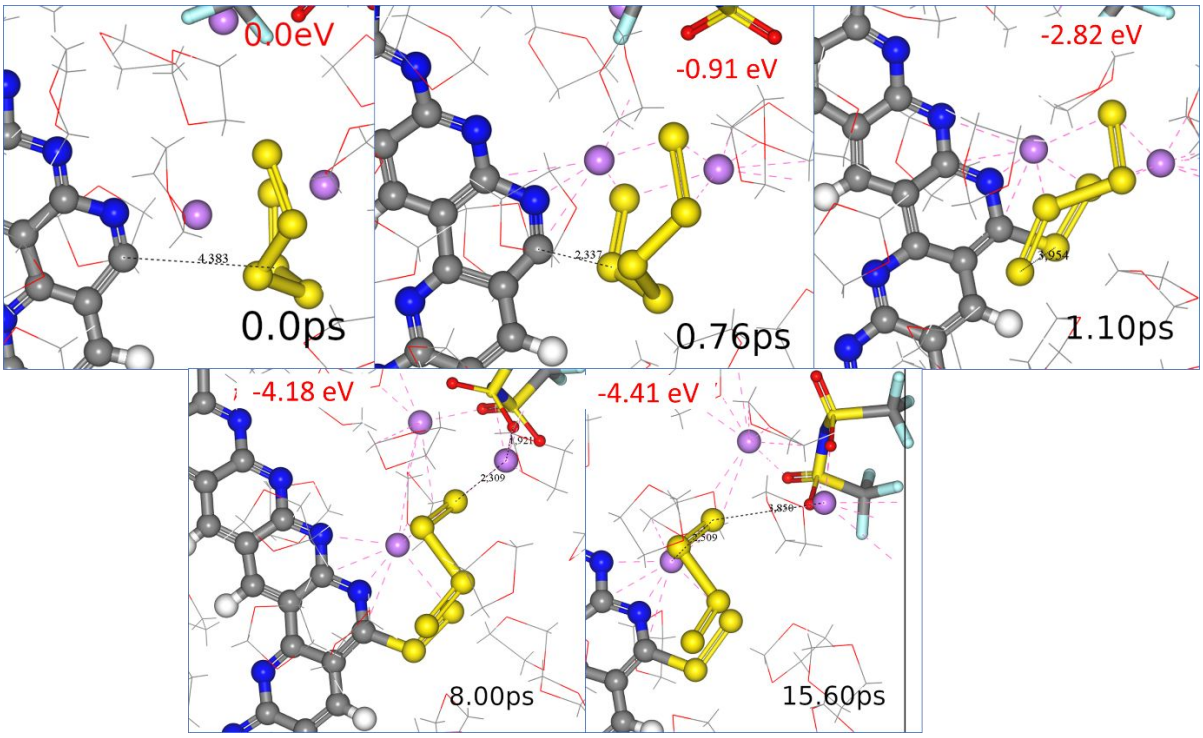

Figure S2: Configuration of the AIMD over time, the system that contains the PS and LiTFSI, where PS is not attached, but it is close to the C_{uc}.

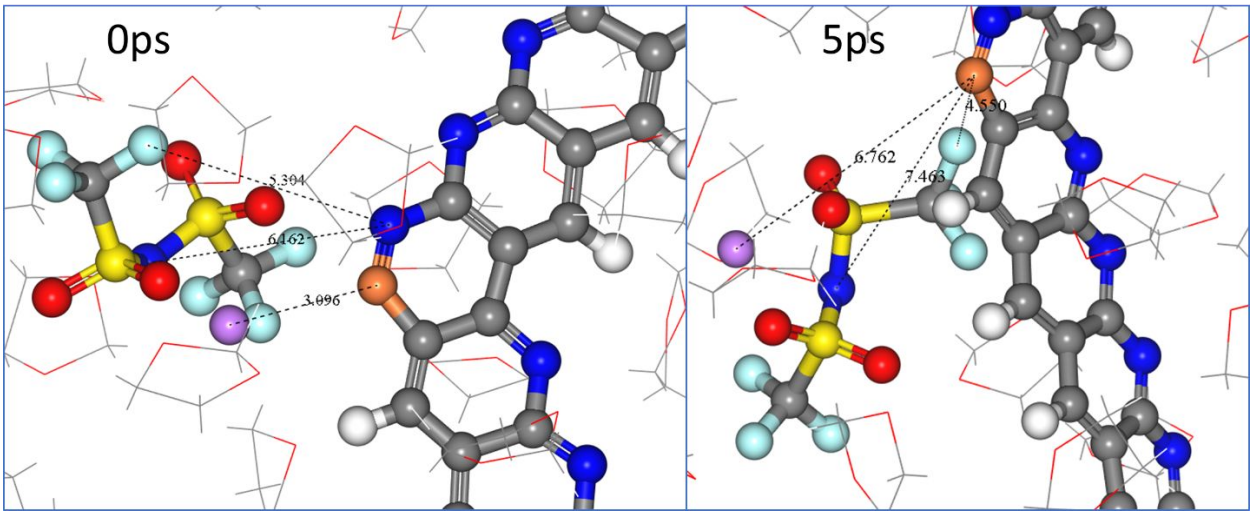

Figure S3: Ab Initio Molecular dynamics when LiTFSI is initially set close to the empty site. The color code is described in **Figure 1**, but the empty site is highlighted in orange.

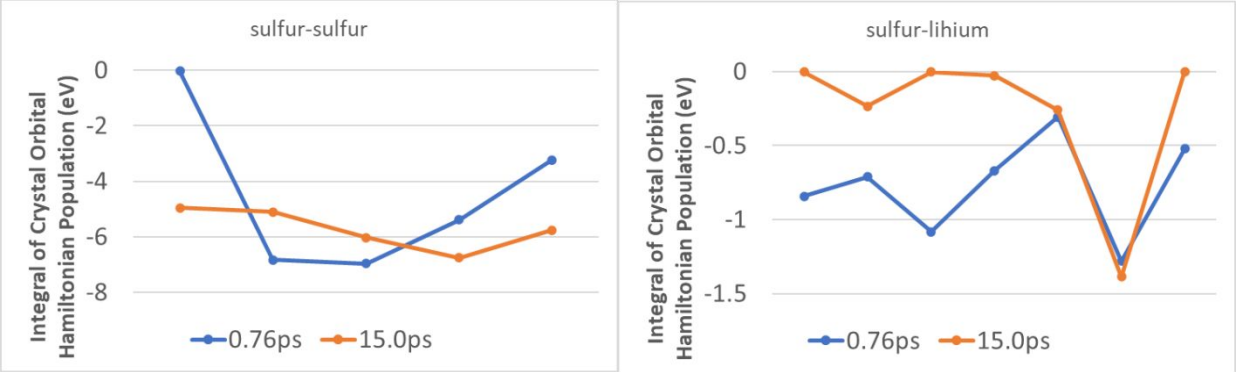

Figure S4: Integral of the Crystal Orbital Hamiltonian Population of C-H bonds that belongs to the system represented in **Figure 1a**.