Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

A Solid Electrolyte Interphase to Protect the Sulfurized Polyacrylonitrile (SPAN) Composite for Li-S Batteries: Computational Approach Addressing the Electrolyte/SPAN Interfacial Reactivity

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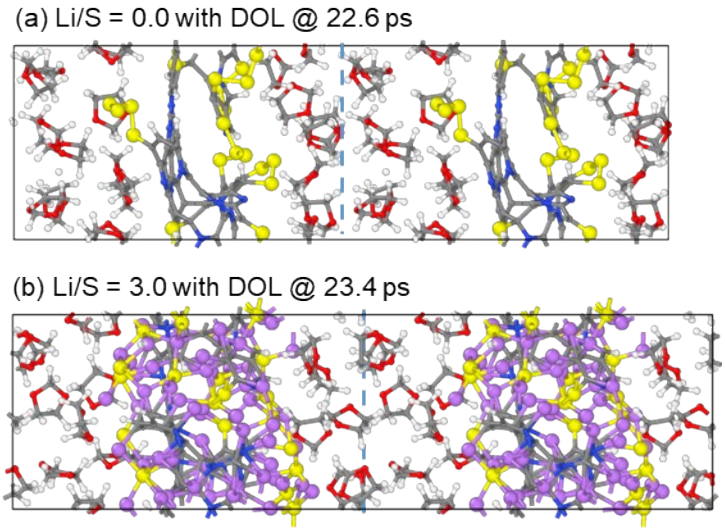

Figure S1: DOL/SPAN interfacial AIMD simulations: (a) Li/S = 0.0, (b) Li/S = 3.0. Color code for atoms as in Figure 2.

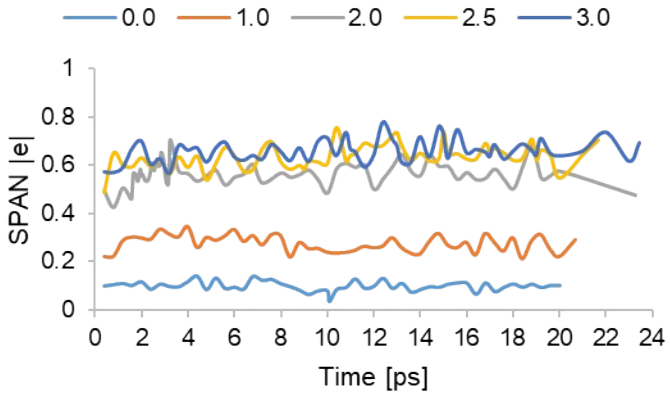

Figure S2: Time evolution of the SPAN surface electronic charge with increasing Li/S molar ratios. DOL/SPAN interfacial interaction.

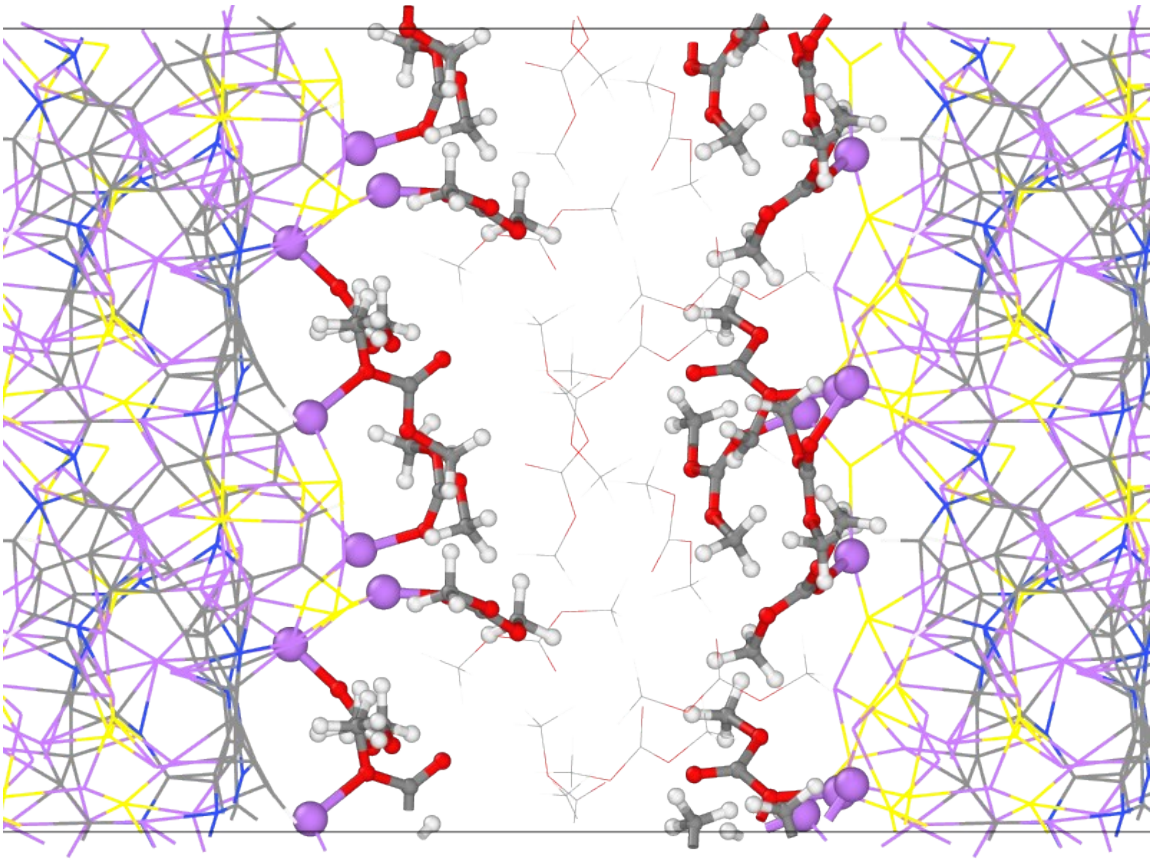

Figure S3: DMC interaction with the lithiated SPAN surface with a 3.0 Li/S molar ratio. Color code for atoms as in Figure 2.

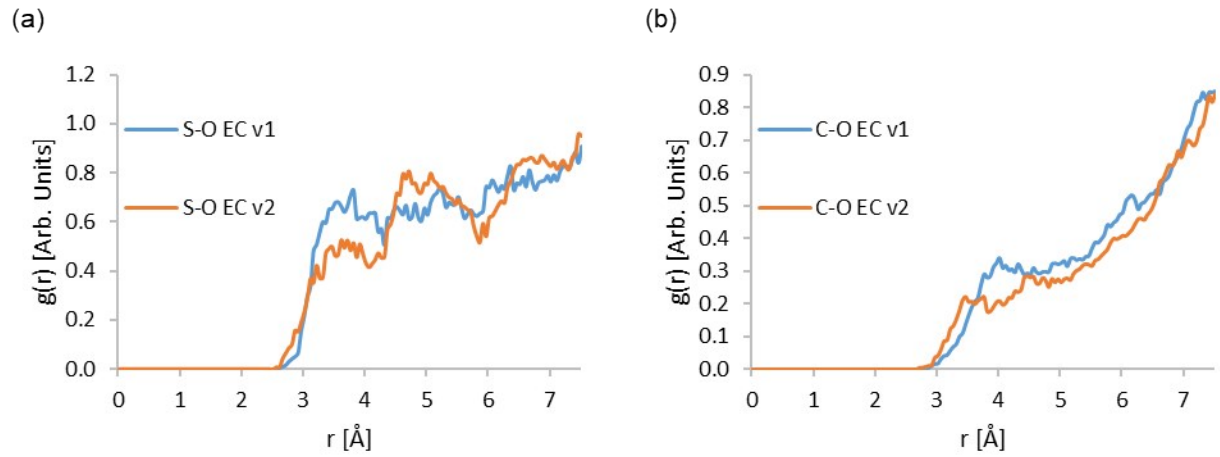

Figure S4: Partial radial distribution function (PRDF) for (a) S-O and and (b) C-O and interactions for the EC interfacial interactions with the SPAN surface before lithiation.

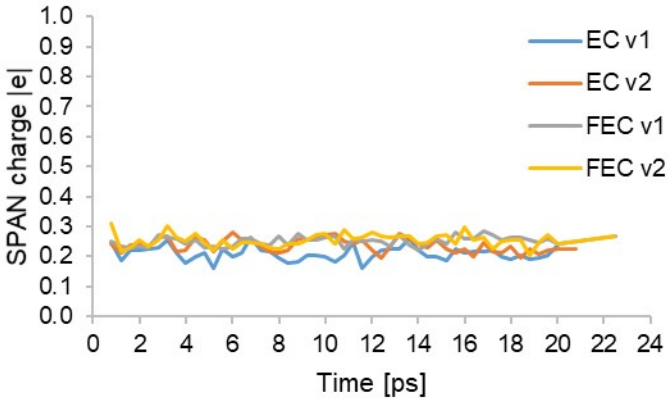

Figure S5: Time evolution for the SPAN electronic charge before lithiation: Simulations with EC and FEC.

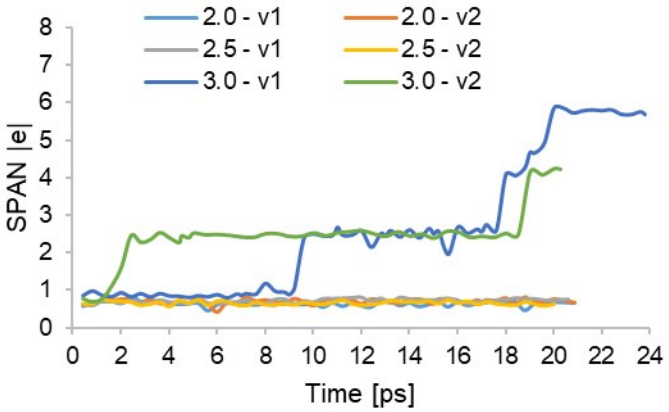

Figure S6: Surface charge time evolution for EC with increasing lithium loadings.

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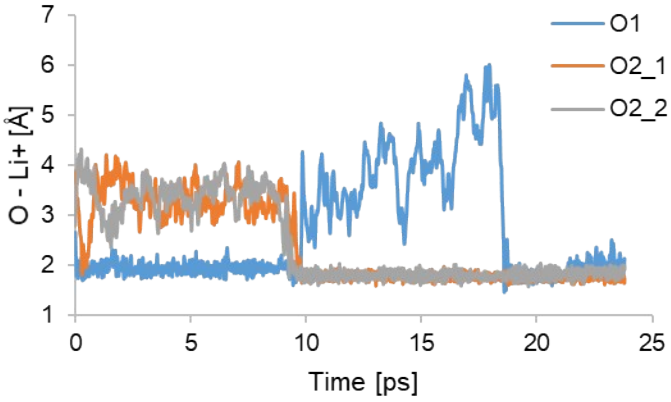

Figure S7: O-Li⁺ distances for 4.ec molecule.

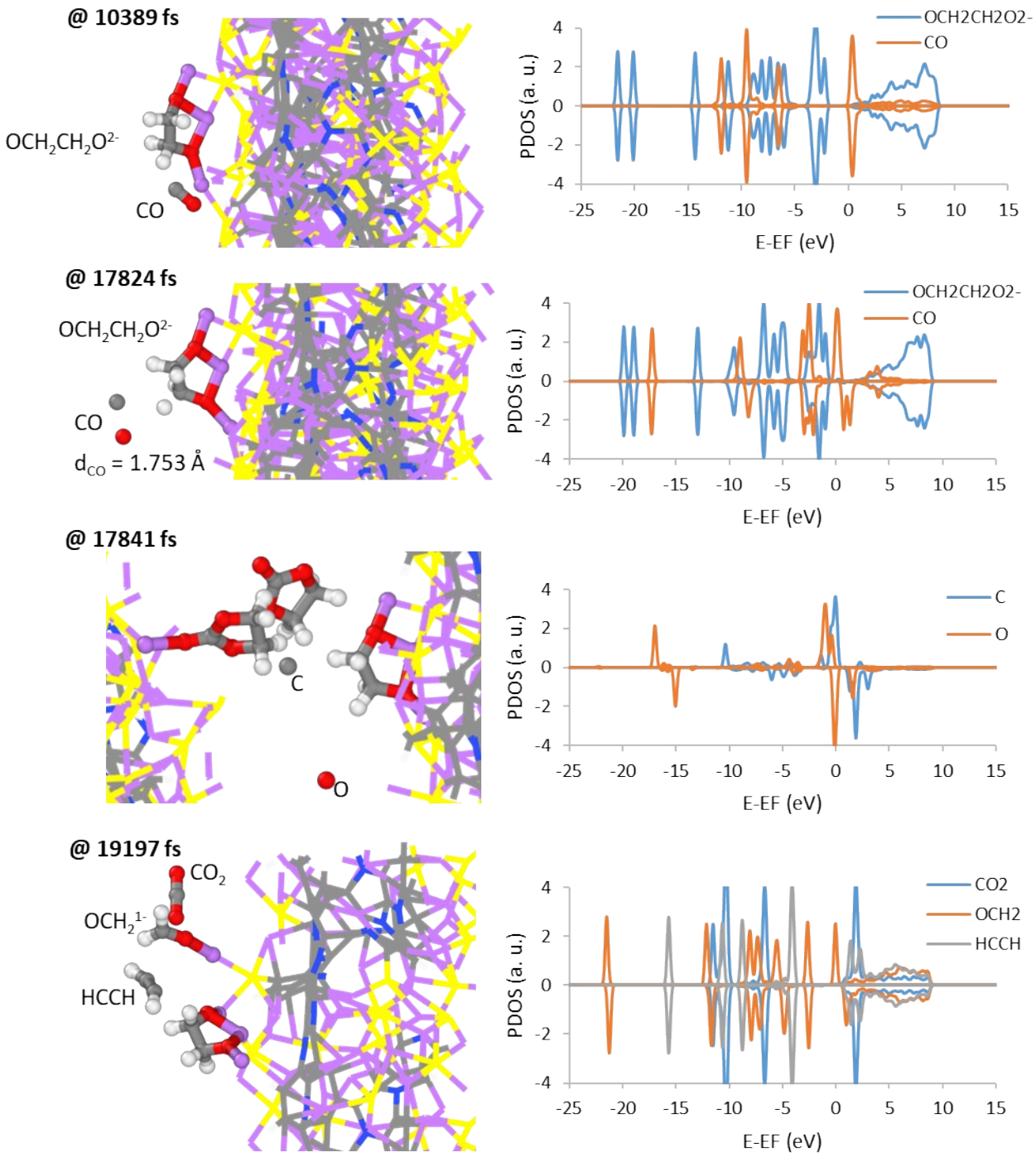

Figure S8: Projected density of states (pDOS) analysis performed on selected frames for the reaction depicted in Figure 8. Color code for atoms as in Figure 2.

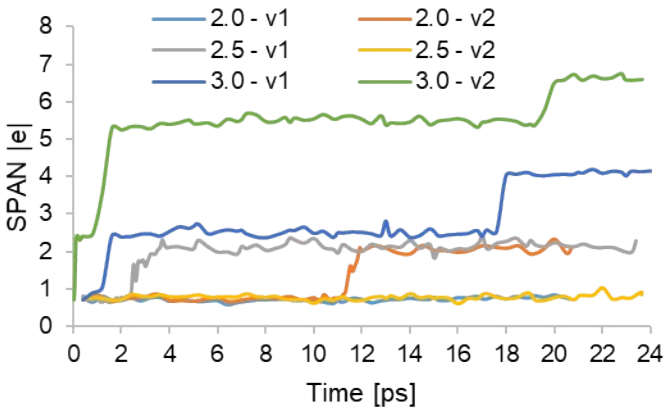

Figure S9: Surface charge time evolution for FEC with increasing lithium loadings.