High voltage lithium ion battery

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a Schematic illustration of SiMPs electrodes cycled in conventional carbonate electrolytes that form silicon-philic organic-inorganic SEI with strong bonding to Si. b Schematic illustration of SiMPs electrodes cycled in the designed electrolytes that form silicon-phobic Li2O-LiF SEI with weak bonding to Si.

The predicted X-ray weighted structure factor from MD simulations for TTE, FEC, SL solvents, and FST electrolytes agreed well with the measured ones further validating our electrolyte structure predictions (Fig.2b). The representative solvates and aggregation of the TTE diluent in the simulation box are shown in Fig.2c and Supplementary Fig.5, indicating the existence of Li+ ion conducting SL-rich and TTE-rich domains.

a-c Typical charge/discharge profiles of the SiMP electrodes cycled in different electrolytes. a FST. b FFT. c EE. d Cycling stability and CEs of SiMPs cycled in FST and reference electrolytes; the cycle rate is C/4 with the first formation cycle at C/20. Source data are provided as a Source Data file.

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