Supporting Information for

Improving Thermal Conduction across Cathode/Electrolyte Interfaces in Solid-State Lithium-Ion Batteries by Hierarchical Hydrogen Bond Network

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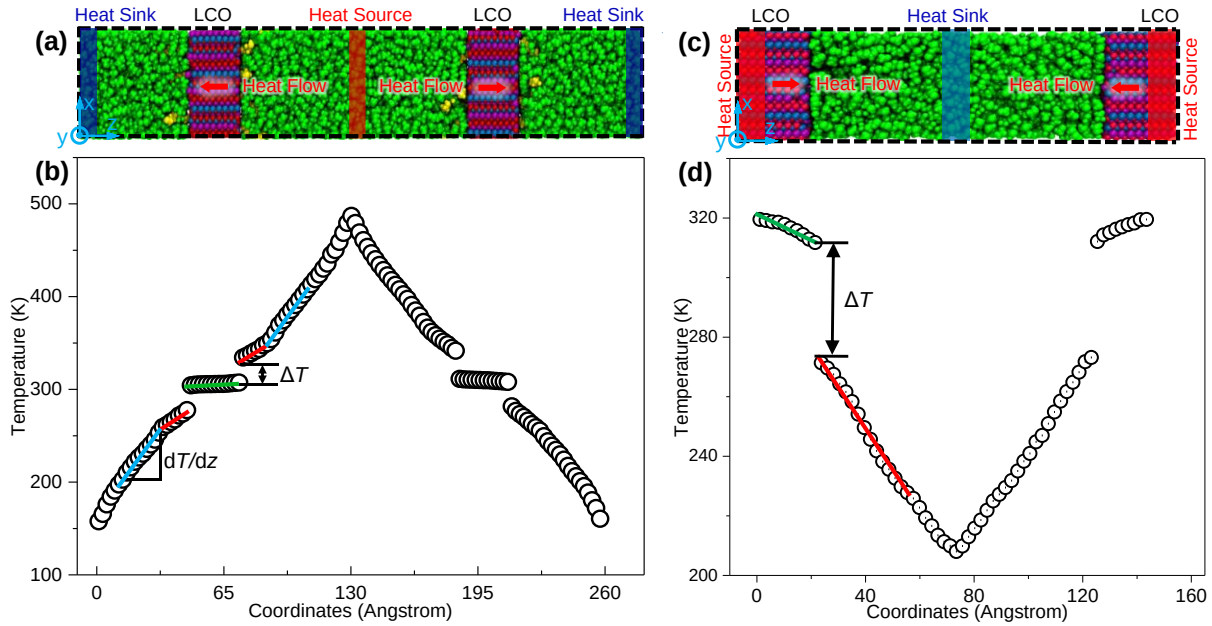

Fig. S1. (a) A simulation system for RNEMD calculation and (b) the associated temperature profile. ΔT is the temperature drop across an LCO/PEO interface, and dT/dz represents the temperature gradient within PEO. (c) A simulation system for NEMD calculation and (d) the associated temperature profile, where the heat source and the heat sink are fixed at 320 K and 210 K, respectively.

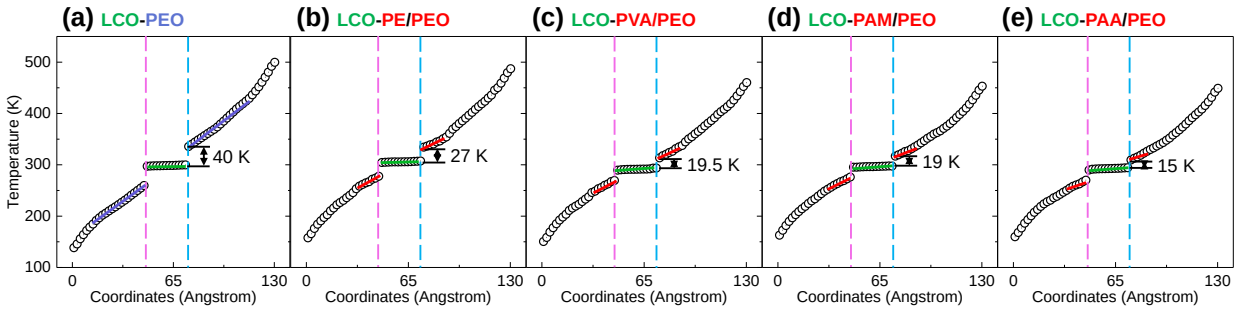

Fig. S2. RNEMD temperature profiles for (a) LCO/PEO, (b) LCO-PE/PEO, (c) LCO-PVA/PEO, (d) LCO-PAM/PEO and (e) LCO-PAA/PEO. Only the left part is shown due to the symmetric simulation system. Between the two vertical dashed lines is the LCO crystal. At the two sides is PEO or PEO with SAM chains.

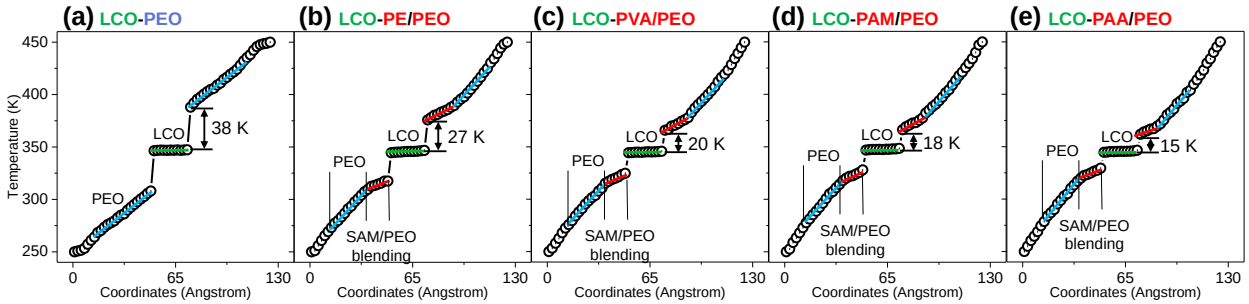

Fig. S3. NEMD temperature profiles of (a) LCO/PEO, (b) LCO-PE/PEO, (c) LCO-PVA/PEO, (d) LCO-PAM/PEO and (e) LCO-PAA/PEO.

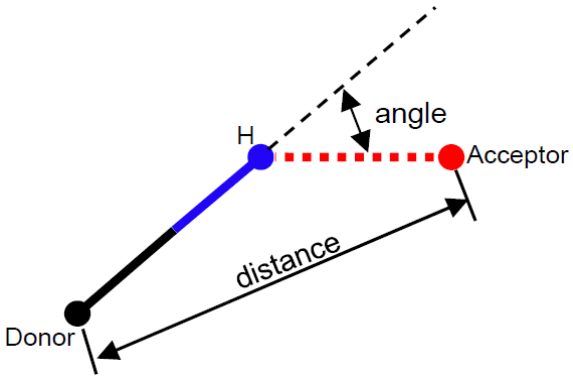

Fig. S4. A H-bond is identified with the following criteria: (1) the distance between the H-bond donor (D) and acceptor (A) is not longer than 3.0 Å; and (2) the angle between H-donor and H-acceptor is not larger than 20˚.