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

Supporting information

Assessing Structure and Stability of Polymer/Lithium-Metal Interfaces from First-Principles Calculations

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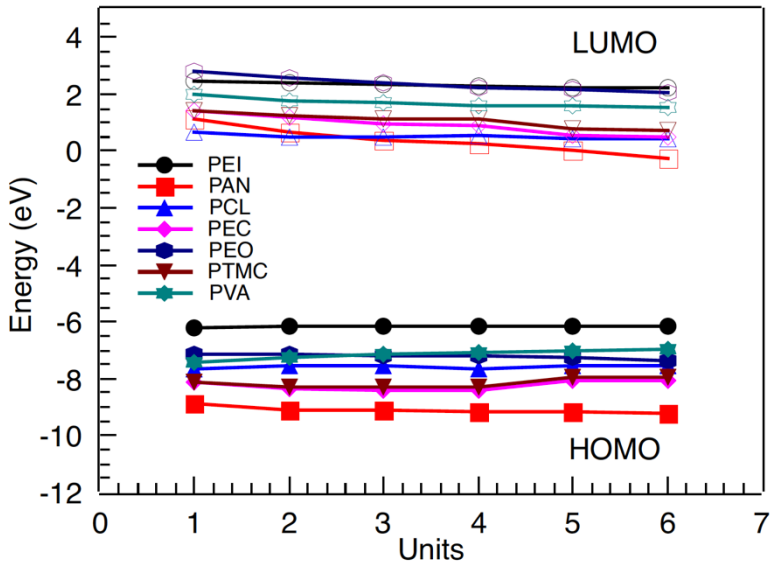
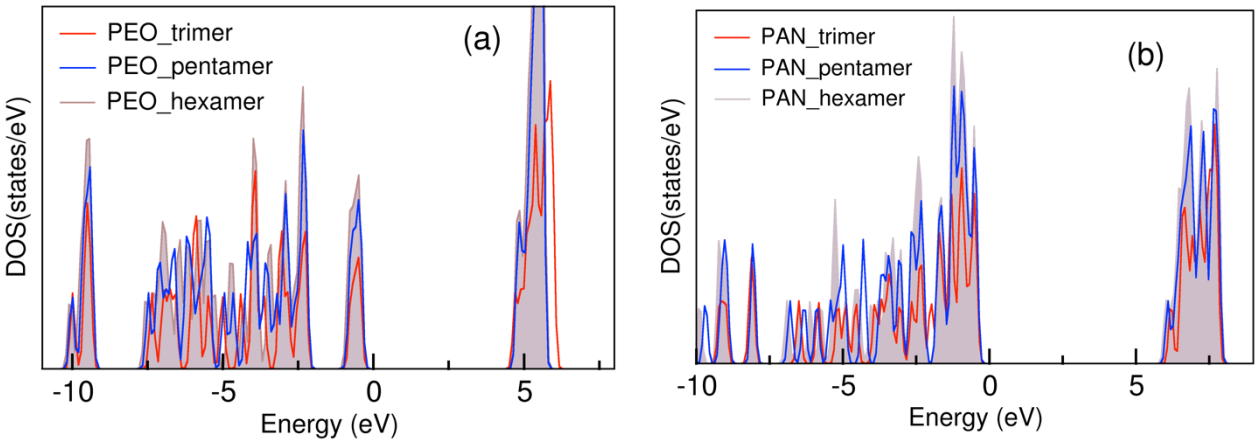


Fig. S1. Highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies for different oligomers in the study with different number of repeating units.



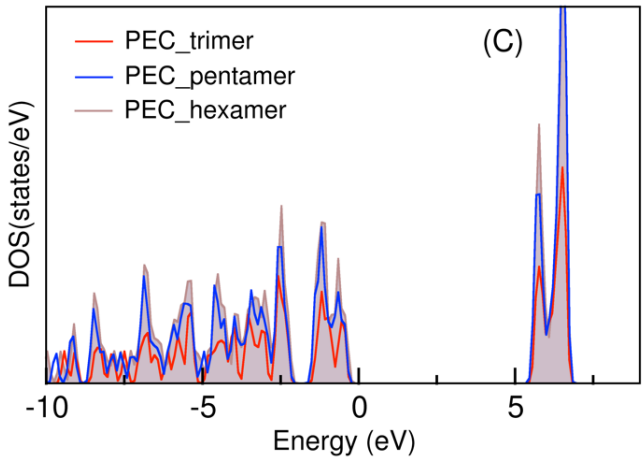


Fig. S2. Total density of states (DOS) of trimer, pentamer and hexamer of (a) PEO, (b) PAN, and (c) PEC.