

Supplementary Material

An Electronic Structure Investigation of PEDOT with AlCl_4^- Anions—A Promising Redox Combination for Energy Storage Applications

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The energy level structure in Figure 8 was based on 6- and 12-PEDOT with anions. The following table shows where the anions are located on the oligomers. These are the lowest energy states found for that number of anions from either a complete sample for 6-PEDOT or large random sample for 12-PEDOT.

Number of anions



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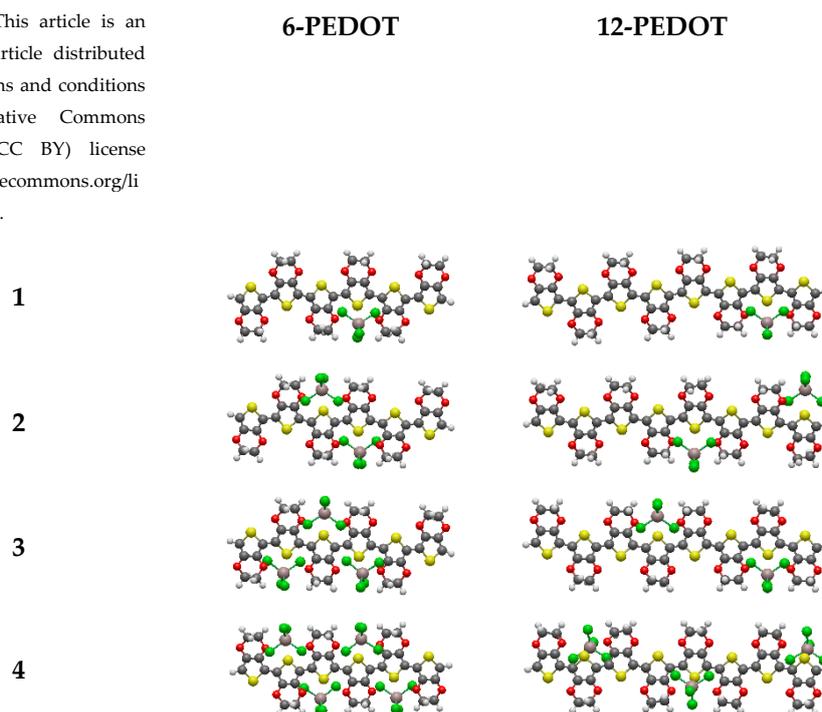


Figure S1. the relaxed configurations of the PEDOT oligomers with anions for which the energy levels are presented in Figure 8. Anions are placed either above or below the oligomer, which can be observed via overlaps in the molecular drawings.