Abstract Submitted
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Photo-oxidation degradation mechanisms in P3HT for organic solar cells: Insights from first-principles simulations[1] KEVIN LEUNG, Sandia National Laboratories, NA SAI, The University of Texas at Austin, JUDIT ZADOR, Sandia National Laboratories, GRAEME HENKELMAN, The University of Texas at Austin — Photo-oxidation is one of the leading chemical degradation mechanisms in polymer solar cells. In this work, using hybrid density functional theory and periodic boundary condition, we investigate reaction pathways that may lead to the sulfur oxidation in poly(3-hexylthiophene)(P3HT) as a step toward breaking the macromolecule backbone. We calculate energy barriers for reactions of P3HT backbone with oxidizing radicals suggested by infrared spectroscopy (IR) and XPS studies. Our results strongly suggest that an attack of hydroxyl radical on sulfur as proposed in the literature is unlikely to be thermodynamically favored. On the other hand, a reaction between the alkylperoxyl radical and the polymer backbone may provide low barrier reaction pathways to photo-oxidation of conjugated polymers with side chains. Our work paves way for future studies using ab-initio calculations in a condensed phase setting to model complex chemical reactions relevant to photochemical stability of novel polymers.

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