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Photoexcitation and Photochemical Stability of Organic Photovoltaic Materials from First Principles[1] NA SAI, The University of Texas at Austin, KEVIN LEUNG, Sandia National Laboratory — The development of high efficiency organic photovoltaics (OPV) has recently become enabled by the synthesis of new conjugated polymers with low band gap that allow light absorption over a broader range of the spectrum. Stability of these new polymers, a key requirement for commercialization, has not yet received sufficient attention. Here, we report first-principles theoretical modeling of photo-induced degradation of OPV polymers carried out using ab-initio density functional theory (DFT). We report photooxidation routes and reaction products for reactive species including superoxide oxygen anions and hydroxyl groups interacting with the standard workhorse OPV polymer, poly(3-hexyl-thiophene) (P3HT). We discuss theoretical issues and challenges affecting the modeling such reactions in OPV polymers. We also discuss the application of theoretical methods to low-band-gap polymers, and in particular, the effect of the chemical substitution on the photoexcitation properties of these new polymers. Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Deparment of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Na Sai
The University of Texas at Austin

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