Novel Polycarbonate Material Design of Light-Resistance: a Theoretical Investigation

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Abstract

We studied the mechanism of polycarbonate (PC) photodegradation using a simplified model bisphenol-A hydrogen carbonate (BPAHC) at first, and the results showed that the PhO-COO- bond cleavage can be explained from two electronic excitations. The well-known one is the electronic excitation from oxygen (within carbonate group) lone pair to the carbonate group that stabilizes the orbital energy of carbonate π anti-bonding, and the newly proposed one is the electronic excitation from oxygen lone pair to phenyl (adjacent to carbonate) group that generates a quinoidal structure; the structure forces Ph=O double bond and induces Ph=O···COO- cleavage.[1]

To further design more novel light-resistant PC materials, on the basis of the above mechanism, the detailed mechanism of photodegradation for donor/acceptor-substituted PCs was investigated with quantum chemical methods with considering the effect of electron-donating and electron-withdrawing groups. The results showed that the PhO-COO- bond cleavage is promoted when introducing the electron-donating group on BPAHC, because the above-mentioned excitations are enhanced, finally generating a quinoidal structure and stabilizing the orbital energy of carbonate π anti-bonding. On the contrary, the PhO-COO- bond cleavage is suppressed when introducing the electron-withdrawing group on BPAHC, because the concentrated excitations are reduced compared to BPAHC.

[1] Xiao Huang, Yuuichi Orimoto, and Yuriko Aoki. Theoretical Analysis of Properties of Ground and Excited States for Photodissociation of the C-O Bond in Polycarbonates. *J. Phys. Chem. A*, 125, 6662-6673 (2021).