Ultraviolet Absorbers in Polymer Studied by Molecular Simulation

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One way to protect polymer coatings against ultraviolet light is to prevent UV absorption. This can be achieved by incorporating UV absorber additives, which preferentially absorb harmful ultraviolet radiation and dissipate it as thermal energy.

We are using molecular simulation to study interactive effects between UV absorbers and local chain environment. Within a polymer, ultraviolet absorbers modify the shape and size distributions of existing free volume holes. Each UV absorber molecule can change conformation, thus polymer-UV absorber interactions within free volume holes can potentially impact ultraviolet absorber functionality. We have observed torsion angle distribution under different conditions (vacuum, liquid, polymer), indicating changes in UV absorber shape.

As a starting point, we have selected oxybenzopheone as a UVA in a polypropylene matrix. Where possible, we use the OPLS force field to describe the interaction between atoms. We then used quantum-mechanics calculations to evaluate some of the missing parameters, particularly partial charges. Missing nonbonded parameters were determined by subdividing the UVA molecule into smaller molecule and comparing predicted properties with experiment.