

Analysis of Ground and Excited State Pair Spatial Localization Towards Understanding the Photodegradation in Polymers

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Photodegradation of polymers is a complex phenomenon that is influenced by both topological and electronic information.¹ Regarding the process of exciting an electron from ground to excited state orbitals for photodegradation to occur, it is known that various relationships need to exist between ground and excited states. Factors between the two states such as oscillator strength and transition energy have been investigated heavily and have shown influence.² Another factor that is believed to effect photodegradation is the spatial localization between the two orbitals relative to each other. To investigate the influence of spatial localization on photodegradation, we employ a cooperative approach between time dependent excited state molecular dynamics (TDESMD) and cheminformatic techniques where topological information is used to help describe the influential path of electron movements.³

References

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