

Substitution Effects Study of an Anoidically Coloring Yellow Electrochromic Material

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Due to the rising interest in electrochromic devices, a DFT/TDDFT method was developed in order to predict the chemical properties and stabilities for a yellow polymer provided by the John Reynolds group. Utilizing the functional-basis set pairing B3LYP/6-31G*, the influence of substituent type and placement coupled with the dihedral angle on the ground state and band gap energies was determined. Herein we report the results of these studies.

