

List of Dissertation Abstract (Department of Environment and Natural Sciences)

Name	Supervisor	Title	Abstract
Hwang Ji-Yong	Matsumoto Shinya	Comparison of semi-empirical and TD-DFT approaches for description of absorption properties of anthraquinone dyes using X-ray crystal structure	<p>Various molecular orbital calculation methods are used in the study of the electronic states of organic dyes. The TD-DFT is frequently used for the calculation of their absorption spectrum, however there are a limited number of publications where the molecular orbitals related to the transition state are discussed in detail in addition to the quantitative evaluation of the absorption wavelength. In this study, I made an attempt to evaluate the applicability of TD-DFT and semi-empirical methods to characterize absorption properties of anthraquinone dyes by using well-analyzed X-ray structure without the optimization step. In addition, the calculated results were examined in detail including the relationship between the absorption properties and geometrical characteristics of anthraquinone molecules.</p>