1O06

# Effect of Organic Dye Compounds on Absorption Spectra of Organic Dye/Anatase (001) System: an Ultra Accelerated Quantum Chemical Molecular Dynamics Study.

○ Chen Lv[1], Kei Ogiya[1], 鈴木 愛[2]、Riadh Sahnoun[1]、古山通久[1]、坪井秀行[1]、畠山 望[1]、遠藤 明[1]、高羽洋充[1]、Carlos Del Carpio[1]、Ramesh C. Deka[2]、久保百司[3]、宮本 明[1,2]

[1]東北大学大学院工学研究科応用化学専攻 (〒980-8579 仙台市青葉区荒巻字青葉 6-6-11-1302)
[2]東北大学未来科学技術共同研究センター (〒980-8579 仙台市青葉区荒巻字青葉 6-6-10)
[3]東北大学大学院工学研究科附属エネルギー安全科学国際研究センター
(〒980-8579 仙台市青葉区荒巻字青葉 6-6-11-701)

## 【Introduction】

The dye-sensitize solar cell (DSSCs) attracted considerable attentions because of potentially low cost. Organic dye sensitizers have been recognized as one of the most important parts for DSSCs to reduce the cost and gain high performance. Because of the diversity of organic dye compounds, computational predication in advance and subsequent synthesis of the ultimately tailor dye sensitizers is an attracting approach to reduce the production cost. However, the high computational cost of conventional computational method limited the study on large-scale/periodic DSSCs. Hence, in the present study, an ultra accelerated quantum chemical molecular dynamics program “New-Colors” was developed based on our original tight-binding quantum molecular dynamics program, “Colors” to explore electronic properties and absorption spectra of organic dye on anatase(001) surface.

## 【Methods】

The ultra-accelerated quantum chemical molecular dynamics program “New-Colors” based on our original “Colors” 1) was developed by our laboratory. Similarly to “Colors” program, the specific atomic parameters, such as valence state ionization potentials and Slater exponent of each atomic orbital, was introduced to “New-Colors” program and around 10,000,000 times acceleration was achieved in compared to the traditional first-principle molecular dynamics method.

## 【Results and Discussion】

The electronic structure, charge, bond population, density of states of PAA was investigated by using “New-Colors” program and DFT method, respectively. A 2.65 eV band gap was achieved by “New-Colors” calculation, which is very close to previous theoretical data [2]. As active dye sensitizer, the electronic absorption spectrum of PAA is of importance. Hence, the “New-Colors” program was performed to explore the electronic absorption spectrum of PAA. The first absorption shown in Fig. 1 can be observed around 469 nm. This result is very close to previous theoretical work [2]. Moreover, the absorption mode and absorption spectra of optimized PAA/anatase(001) systems were also studied. The absorption edge of PAA/anatase(001) system shows good UV-vis light photosensitization. This result demonstrate that PAA/anatase(001) may be a candidate of DSSCs. Our results conformed that in-house program “New-Colors” is an effectively tool to study spectra properties for both molecular and periodic systems.

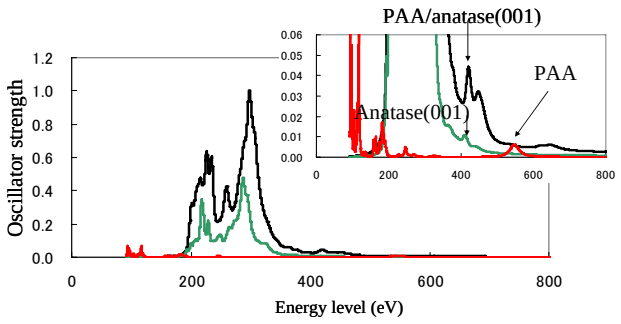


Fig. 1 UV-vis absorption spectrum PAA/anatase(001) system.

**References:**

1. T. Yokosuk et al., Jpn. J. Appl. Phys. **41** (2002) 2410.
2 P. Persson et al., J. Chem. Theory. Comput. **2** (2006) 441.