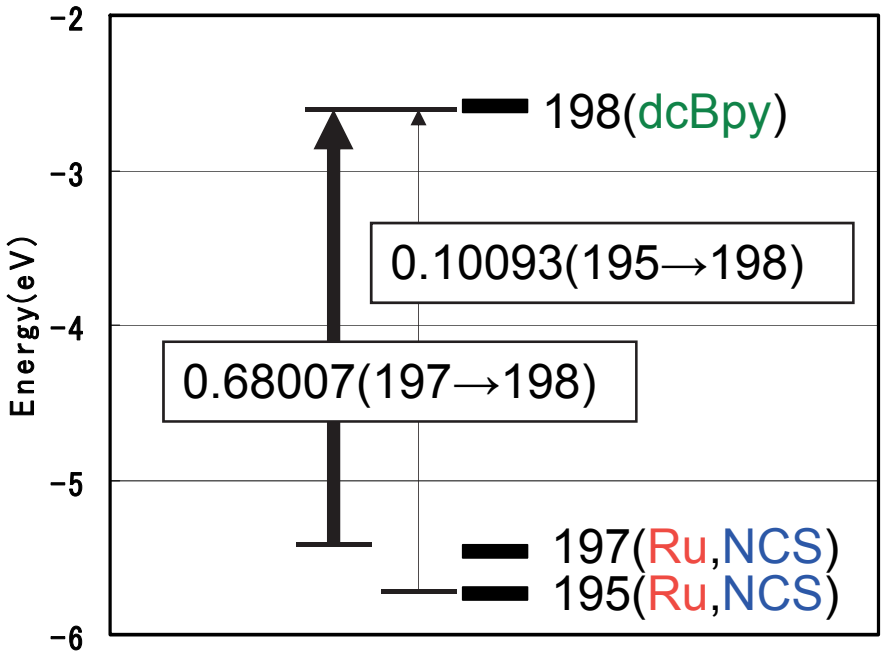
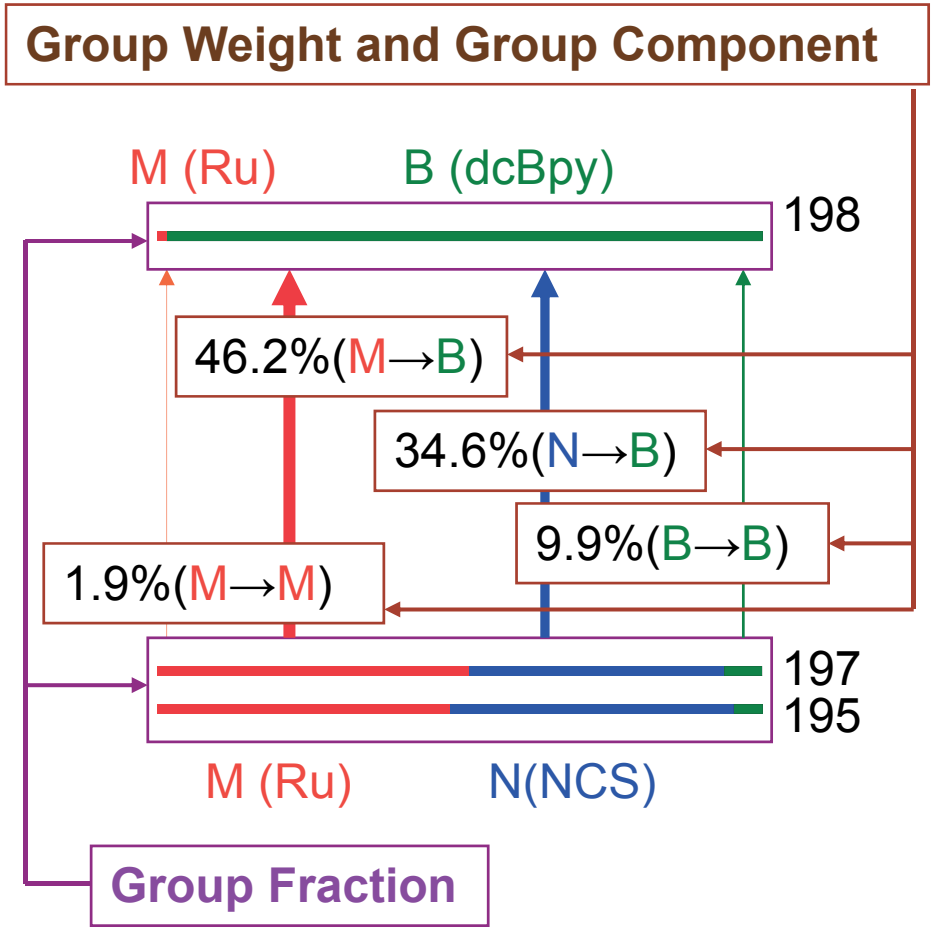
遷移成分解析法による色素増感太陽電池の検討 （革新材料チーム）北尾修



Standard Analysis



TCA (Transition Component Analysis)

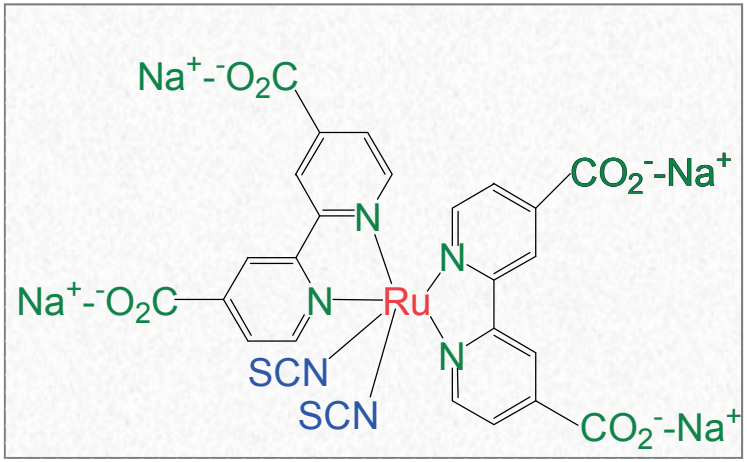
Computational Details (1-4)

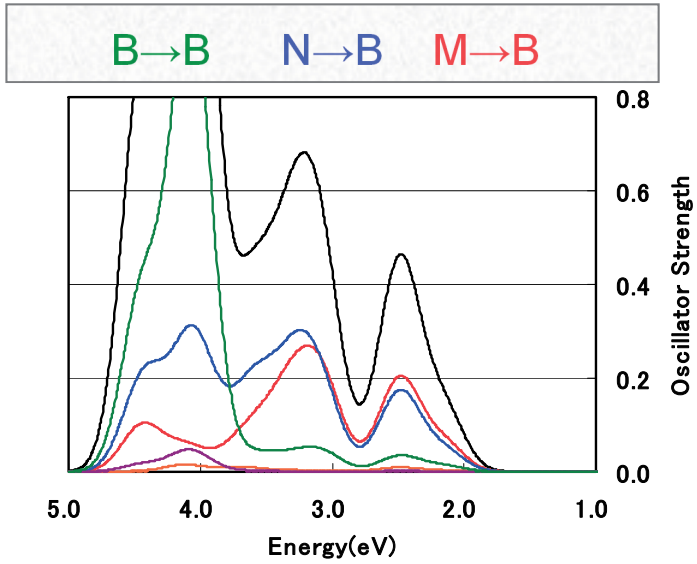
Dye-design System based on TCA (Transition-Component Analysis)

Exchange-correlation Functional Type: B3LYP

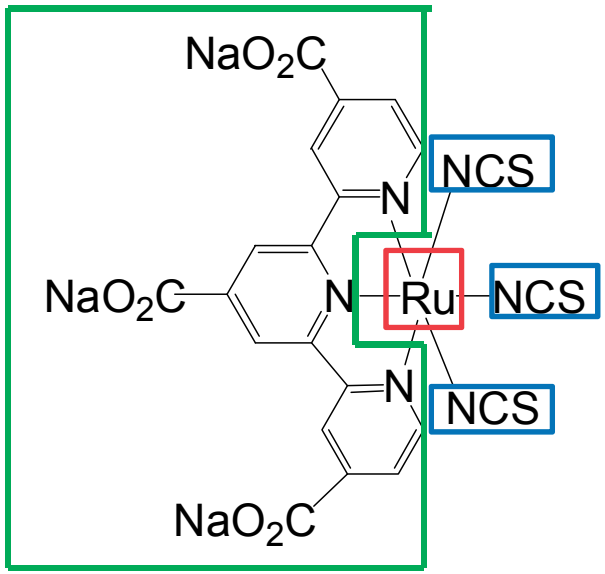
Basis set Type: DGDZVP Solvent: water

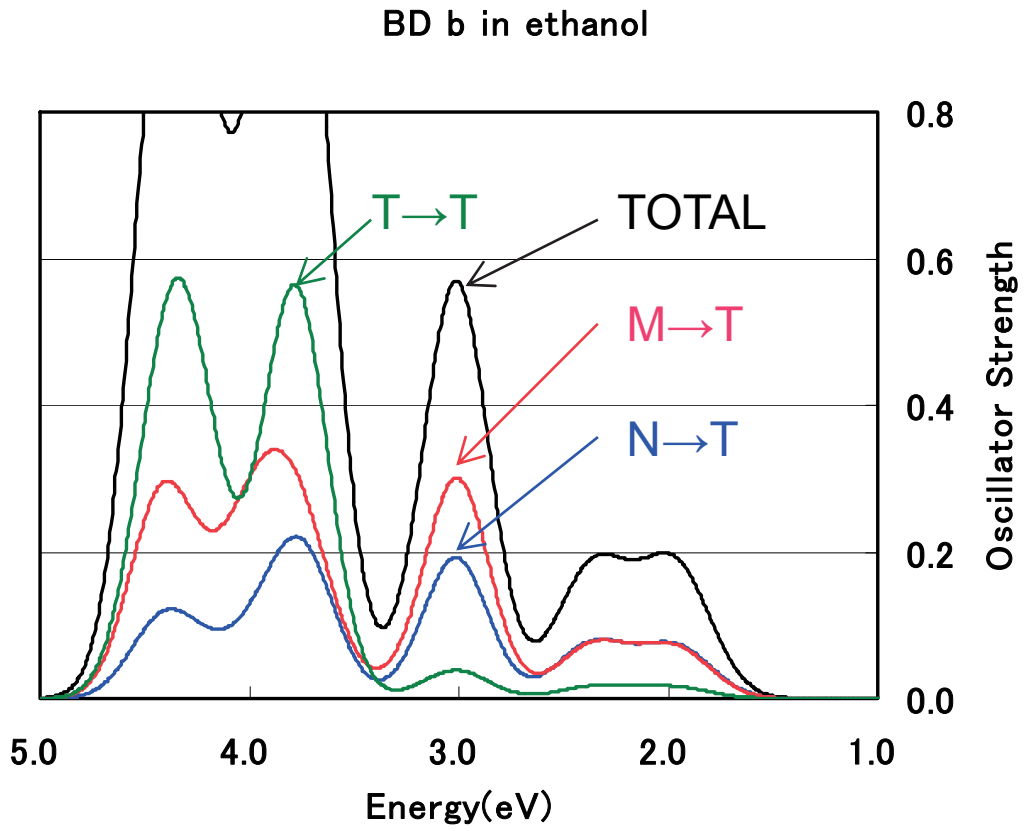
Calculation Step: TCA





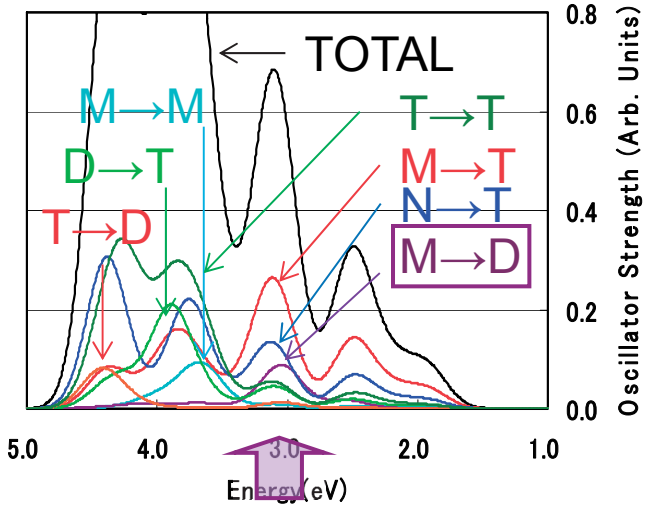
遷移成分解析法の事例(1)

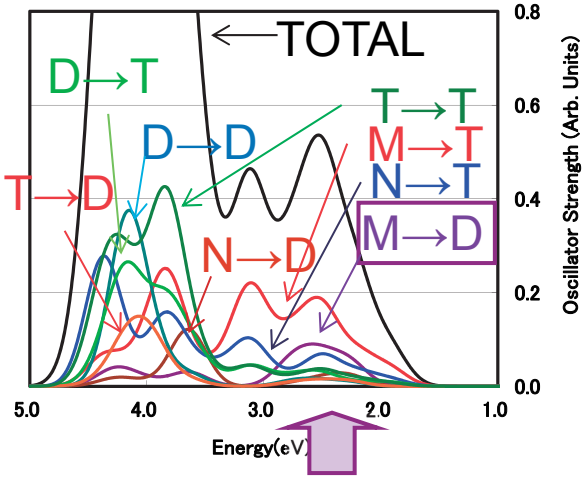


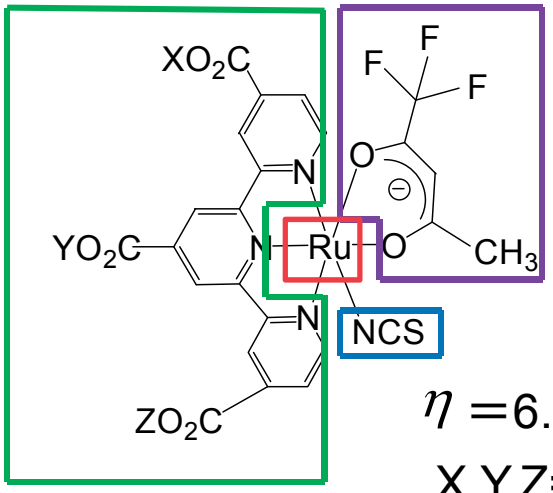


TOTAL (black), M→T (red), T→T (green), and N→T(blue), respectively, where "M" is metal, "N" is NCS, and "T" is tcTerpy.

遷移成分解析法の事例(2)



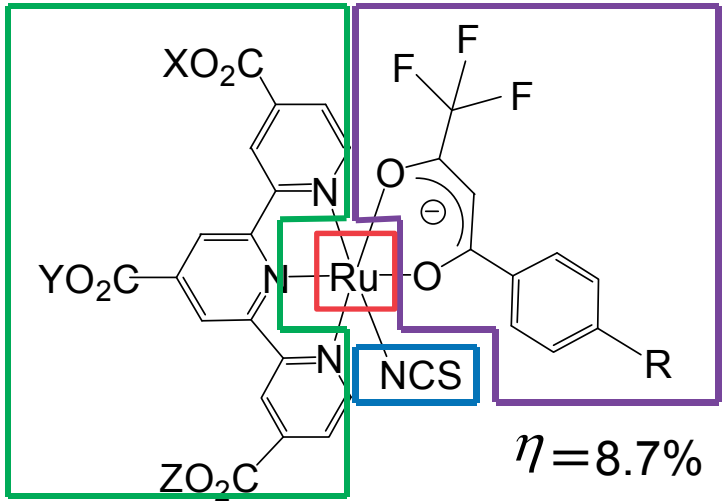




η =6.7%

X,Y,Z=Na

"M" is Metal, "N" is NCS, "D" is Diketonato, and "T" is tcTerpy.



η =8.7%

R=H;X,Y,Z=Na