

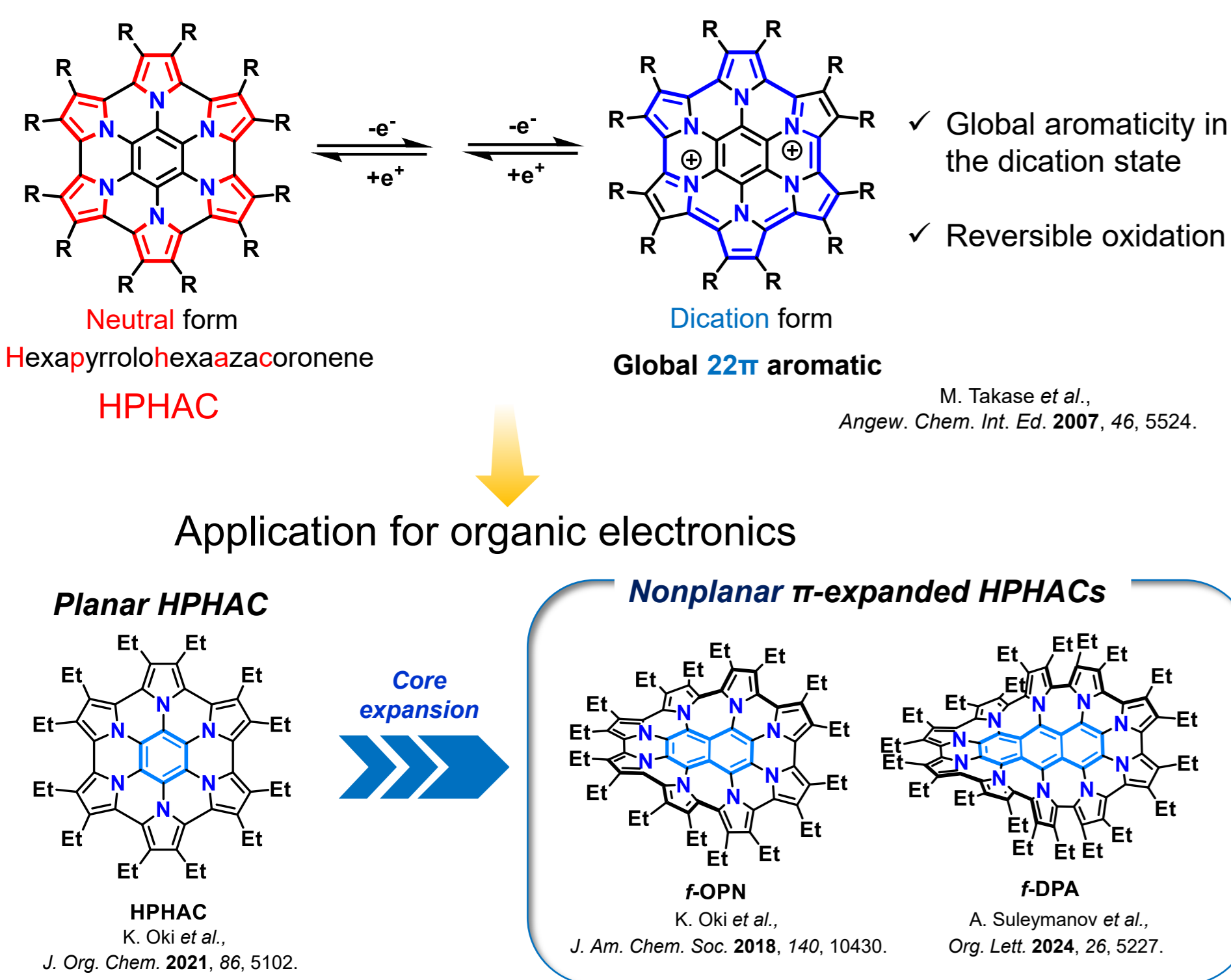


ジベンゾチオフェン骨格を導入した八員環含有 湾曲ナノグラフェンの合成と物性

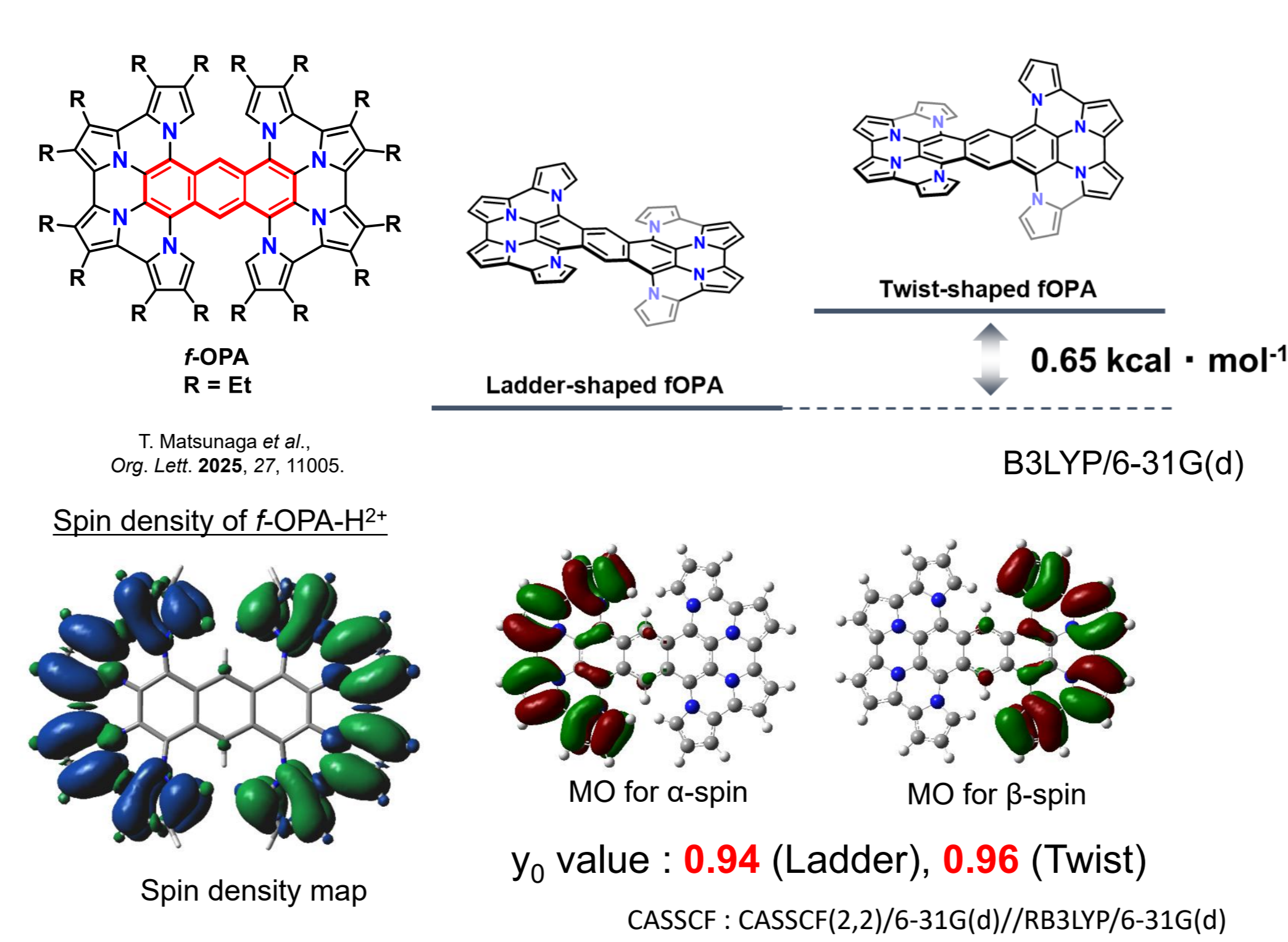
○山本陽太¹, 谷岡雄真², 和多海斗², 森 重樹³, 奥島鉄雄², 宇野英満², 高瀬雅祥²
(愛媛大理¹, 愛媛大院理工², 愛媛大ADRES³)



Introduction



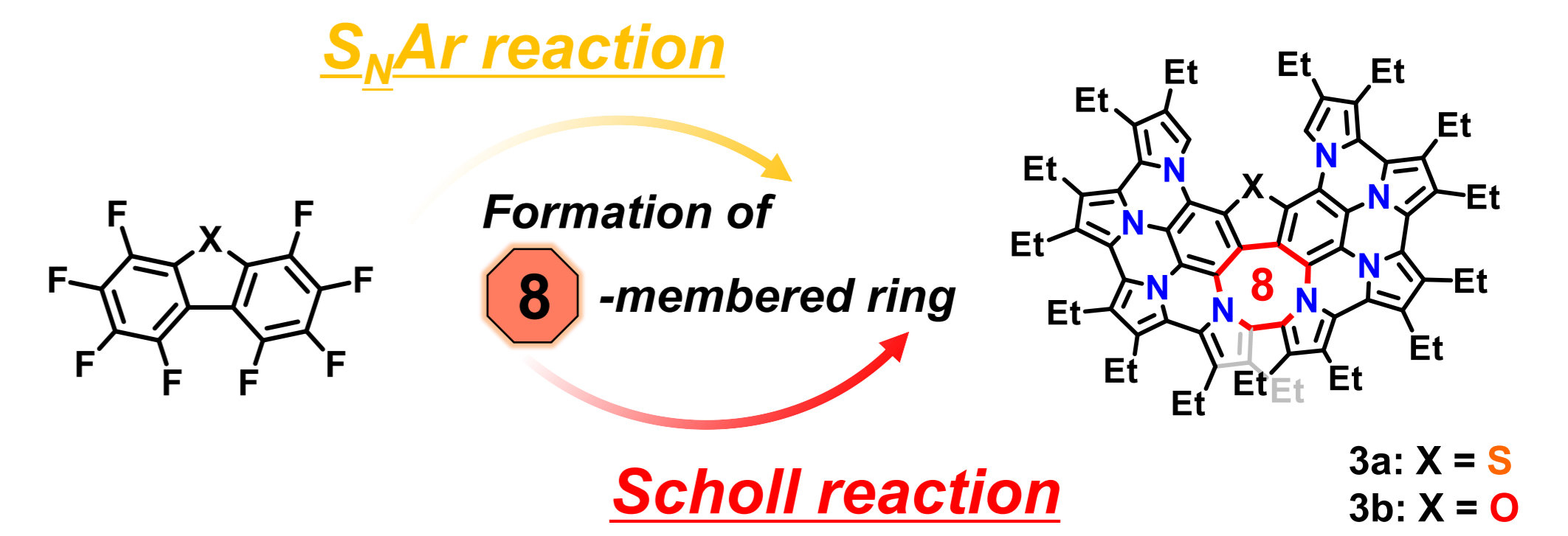
Previous work



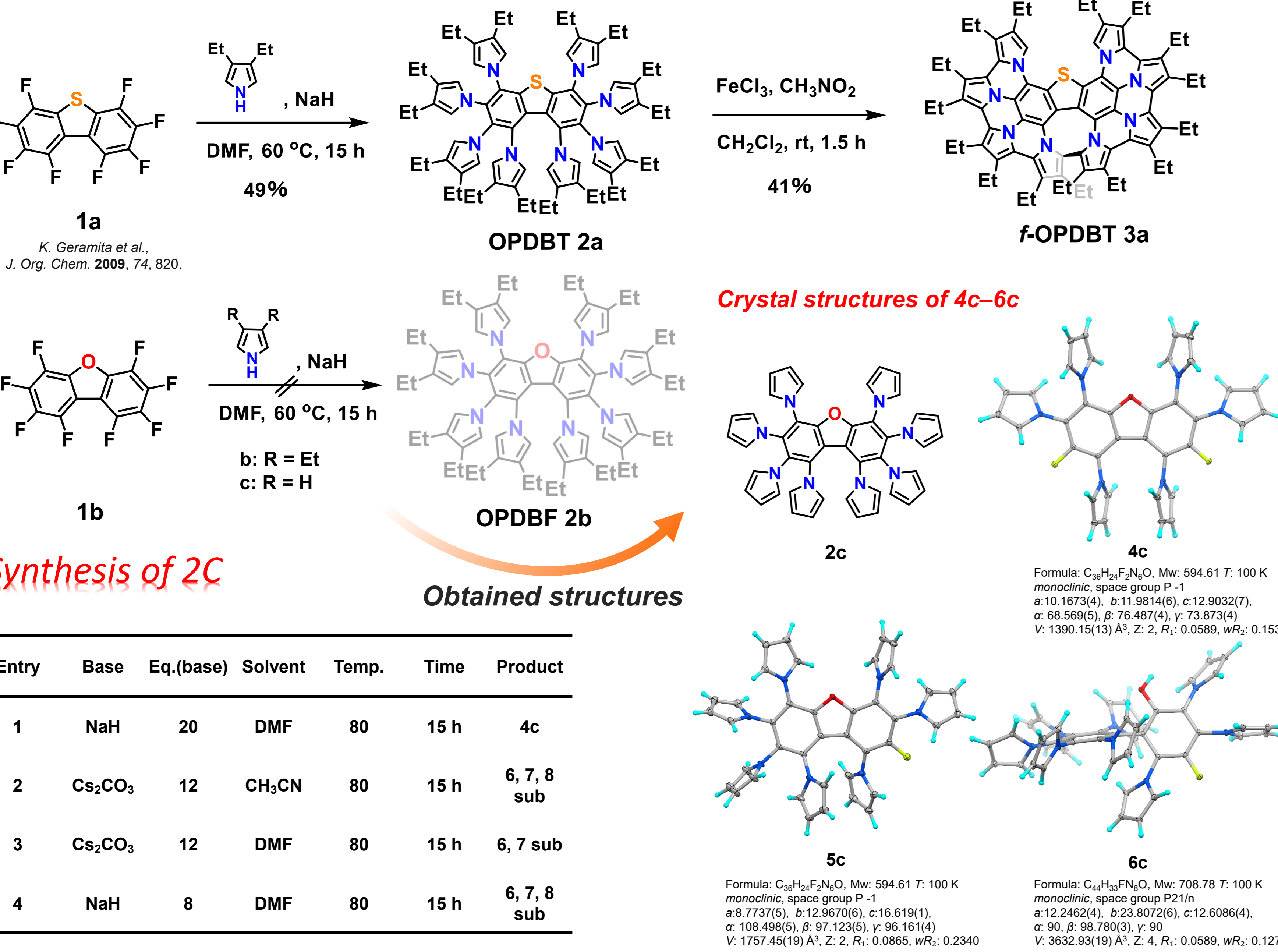
This work

- ◆ Formation of 8-membered ring via S_NAr reaction and Scholl reaction
- ◆ Investigation of structural and physical properties

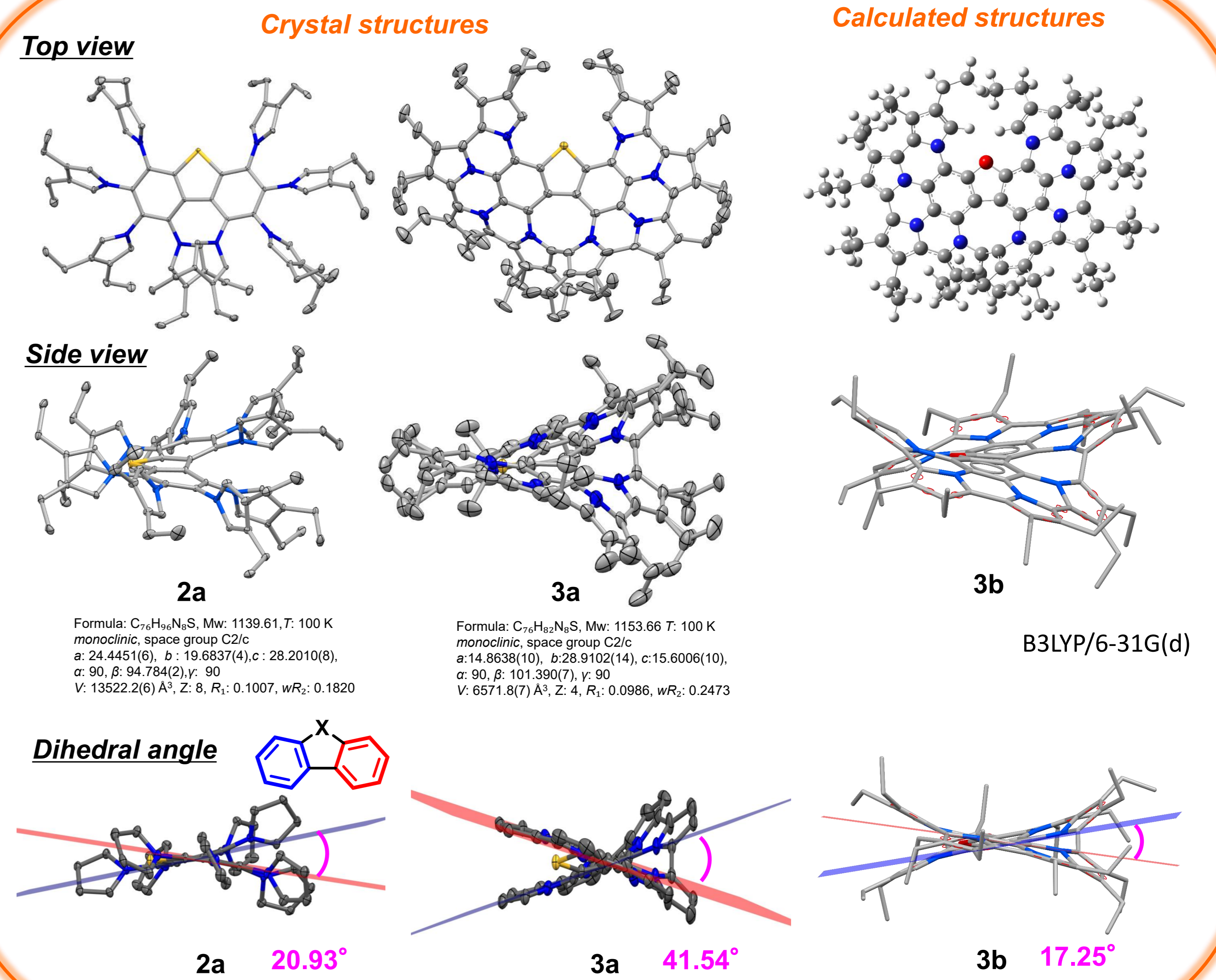
New azacoronene derivative



Synthesis

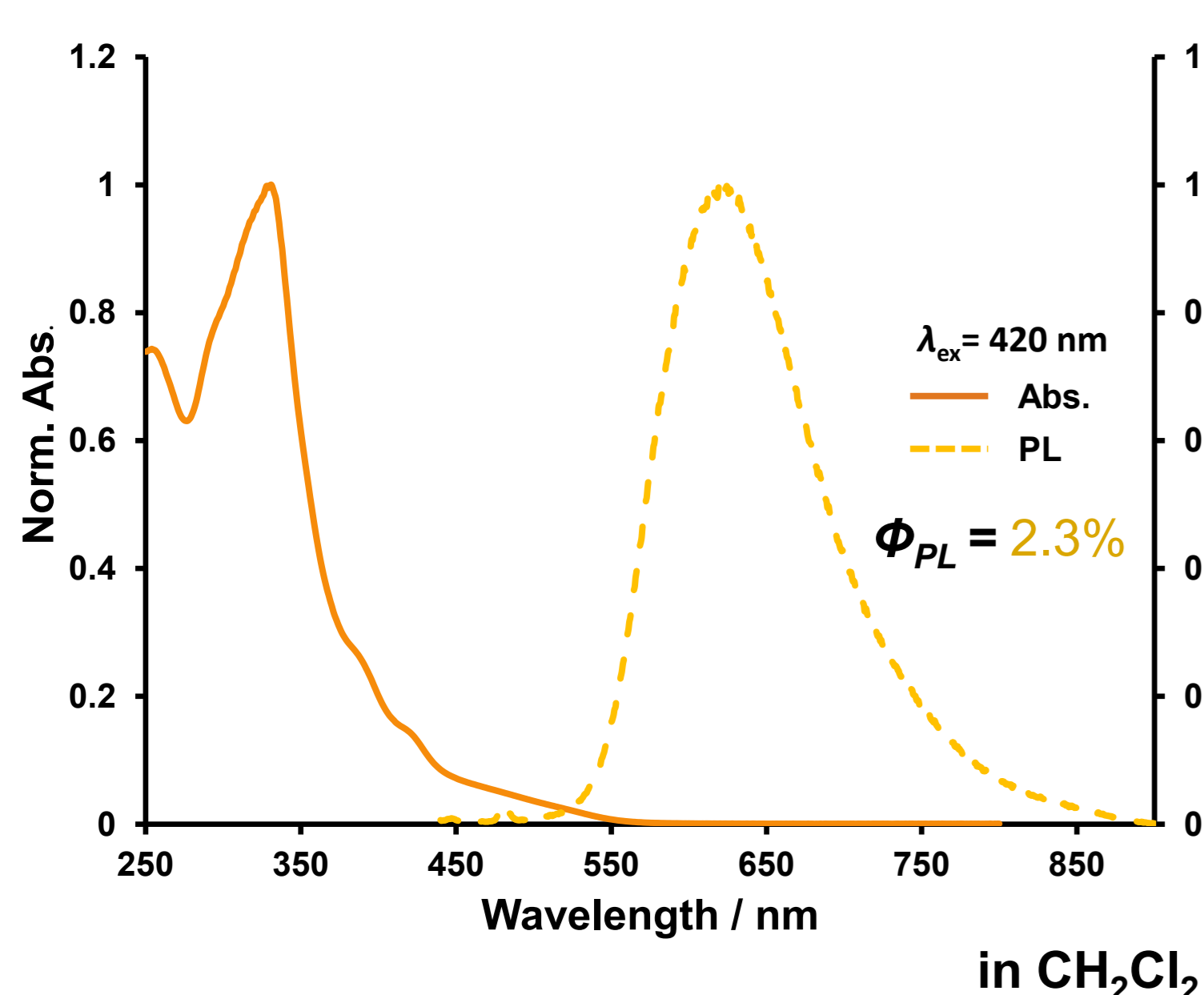


Molecular structures

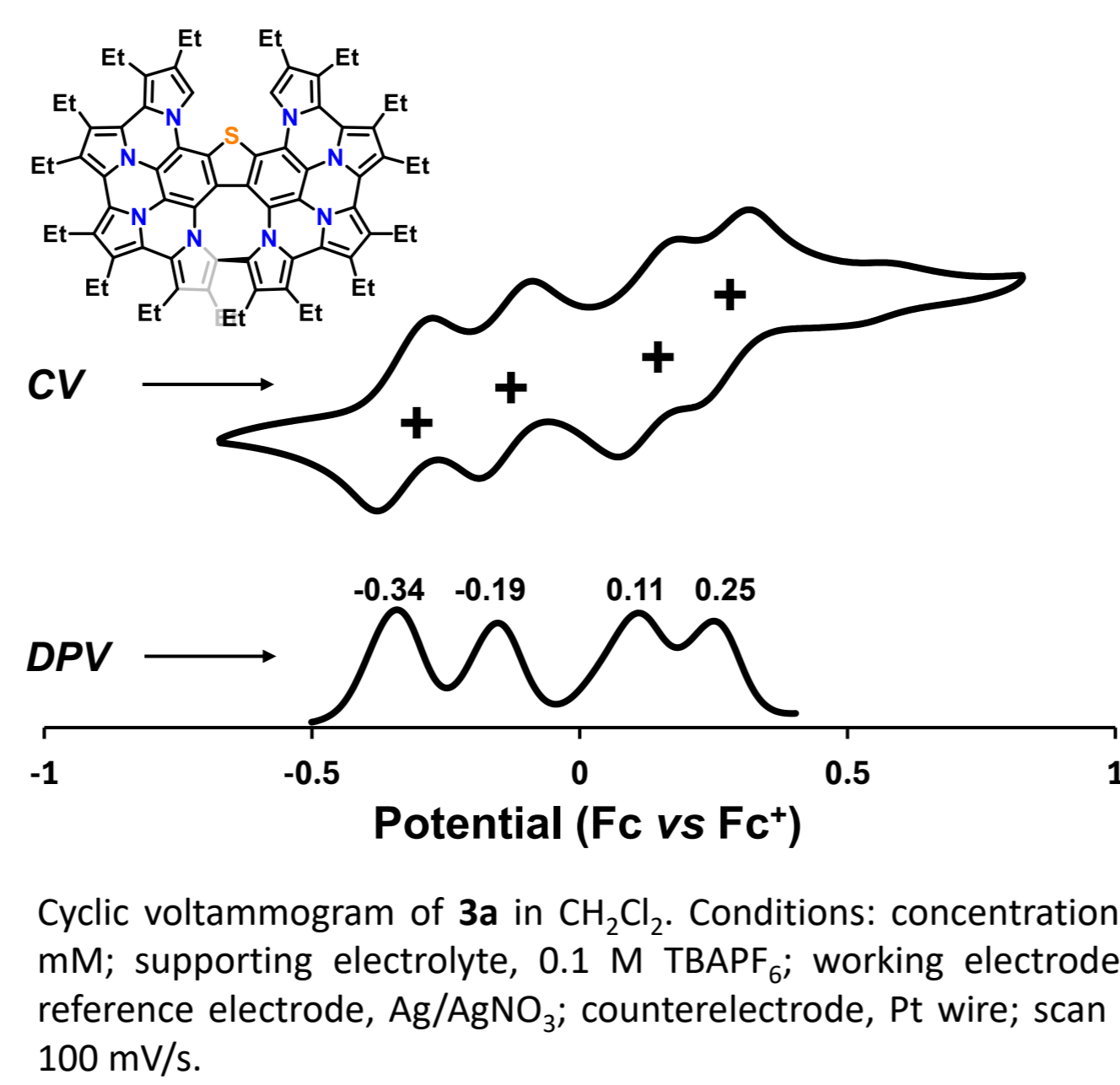


Physical properties

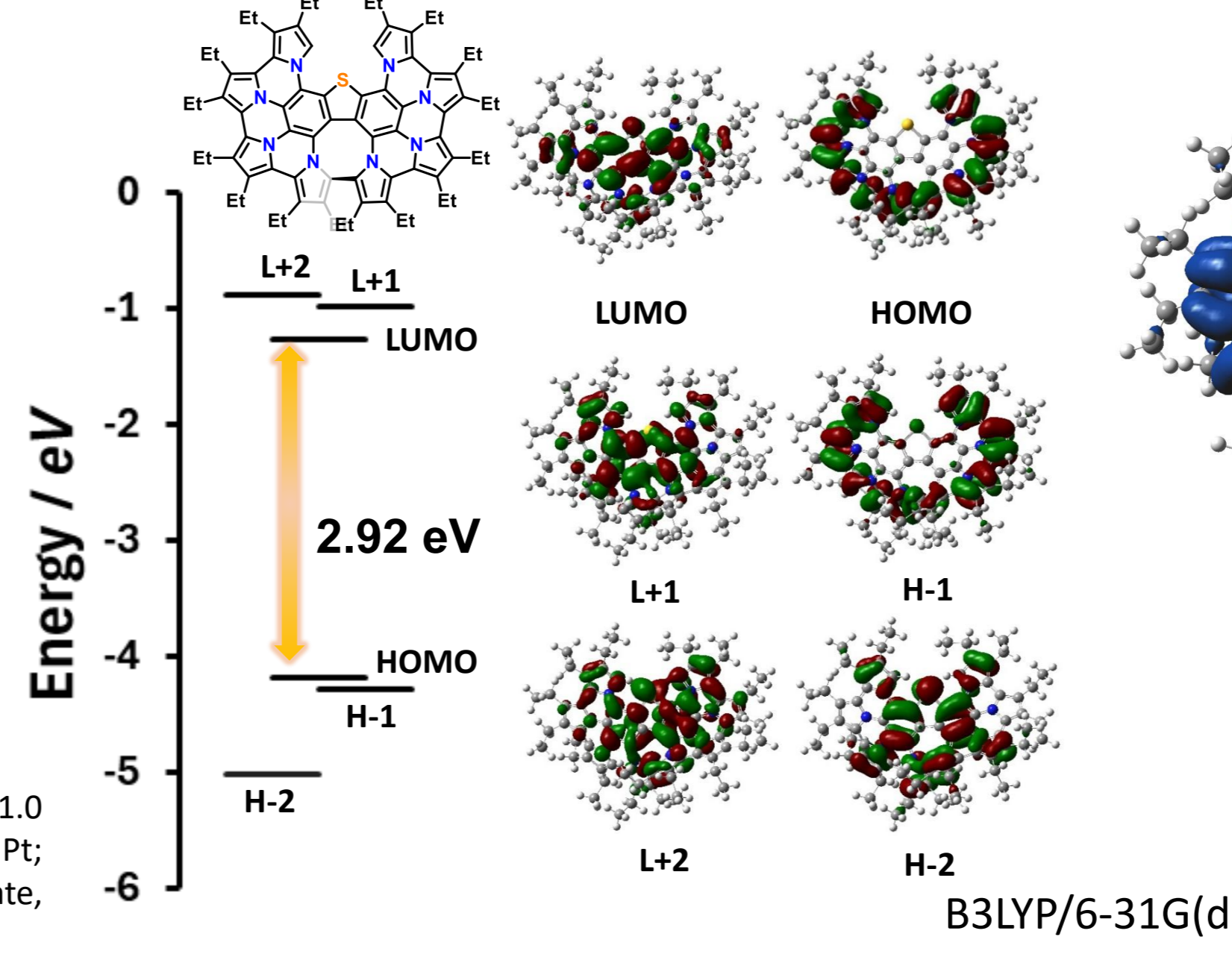
Optical properties of 3a



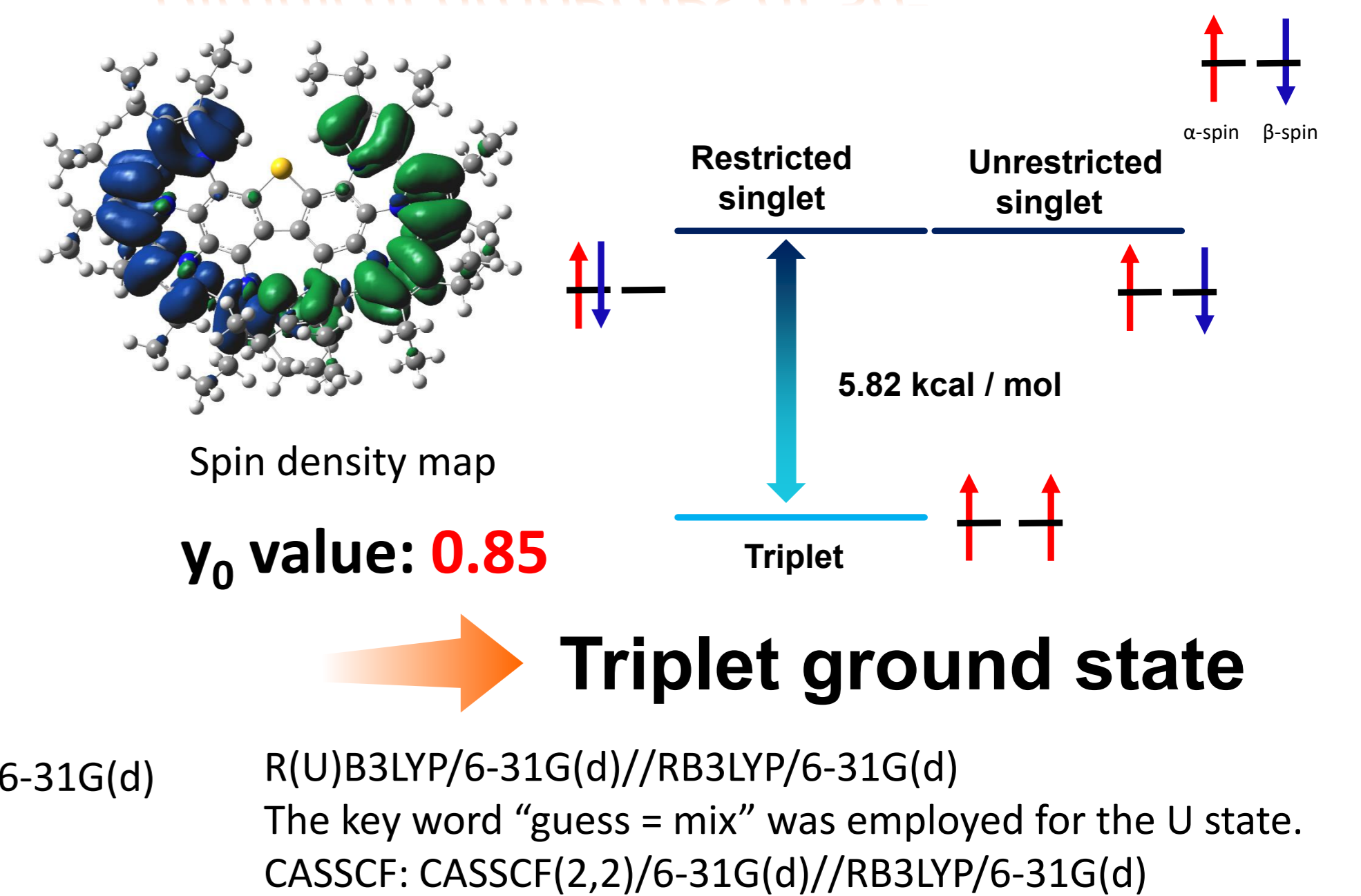
Redox properties



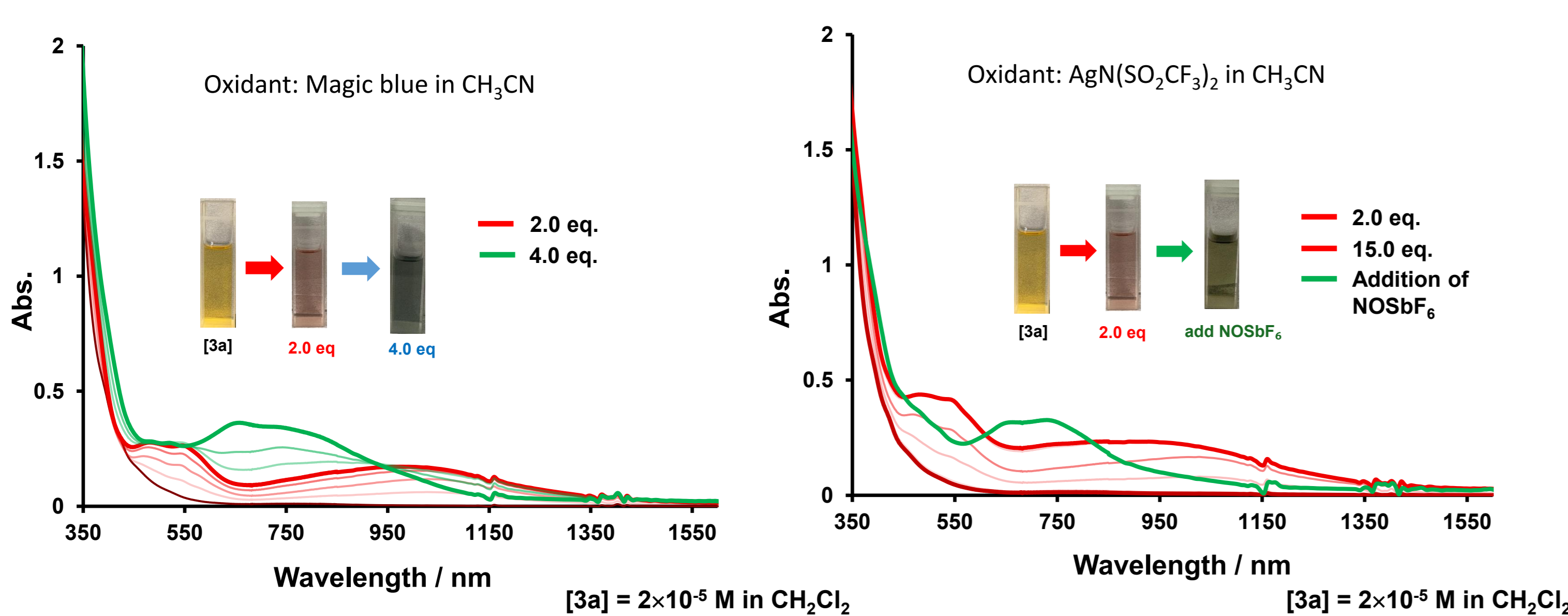
Frontier MOs



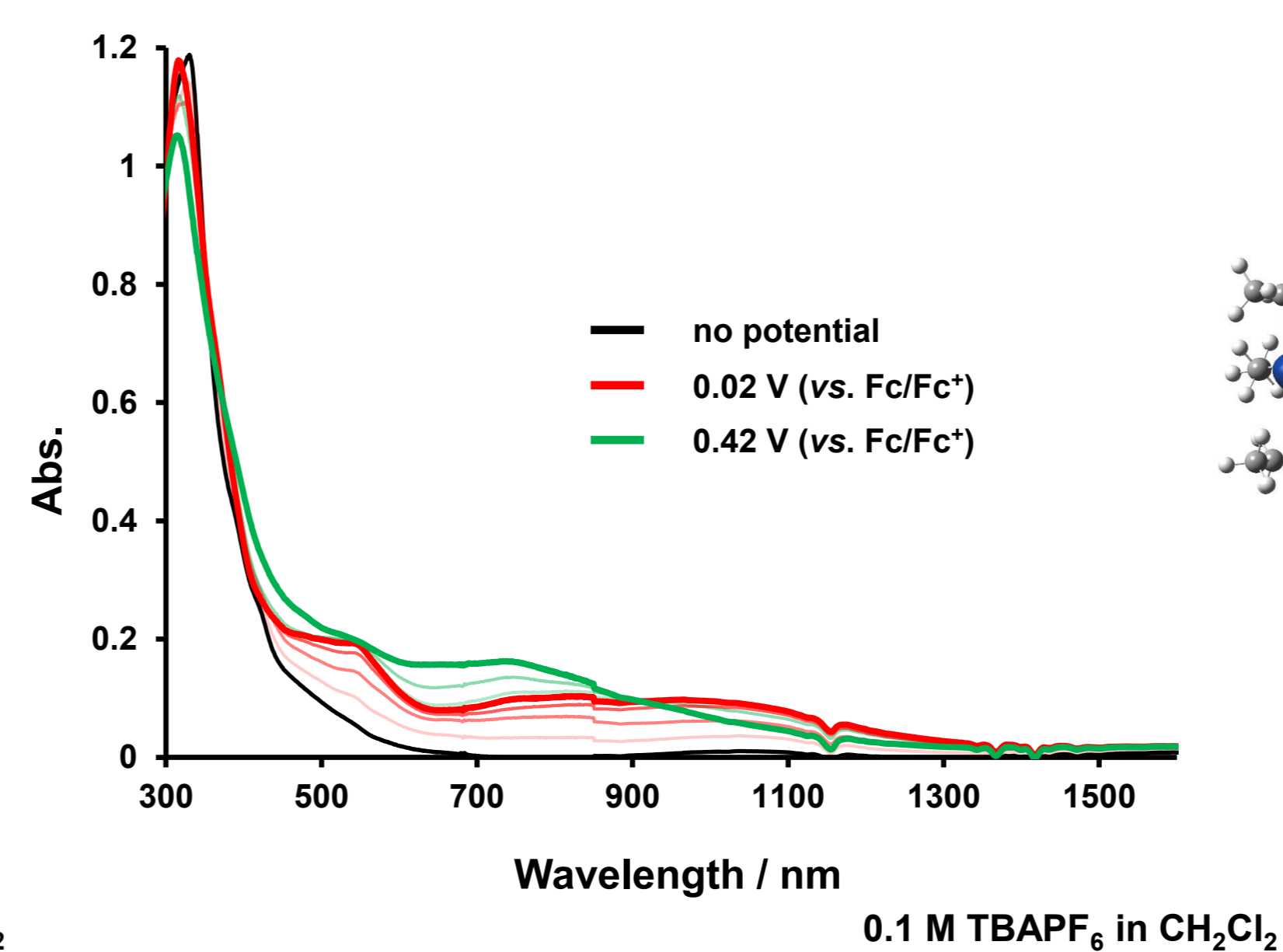
Diradical properties of 3a²⁺



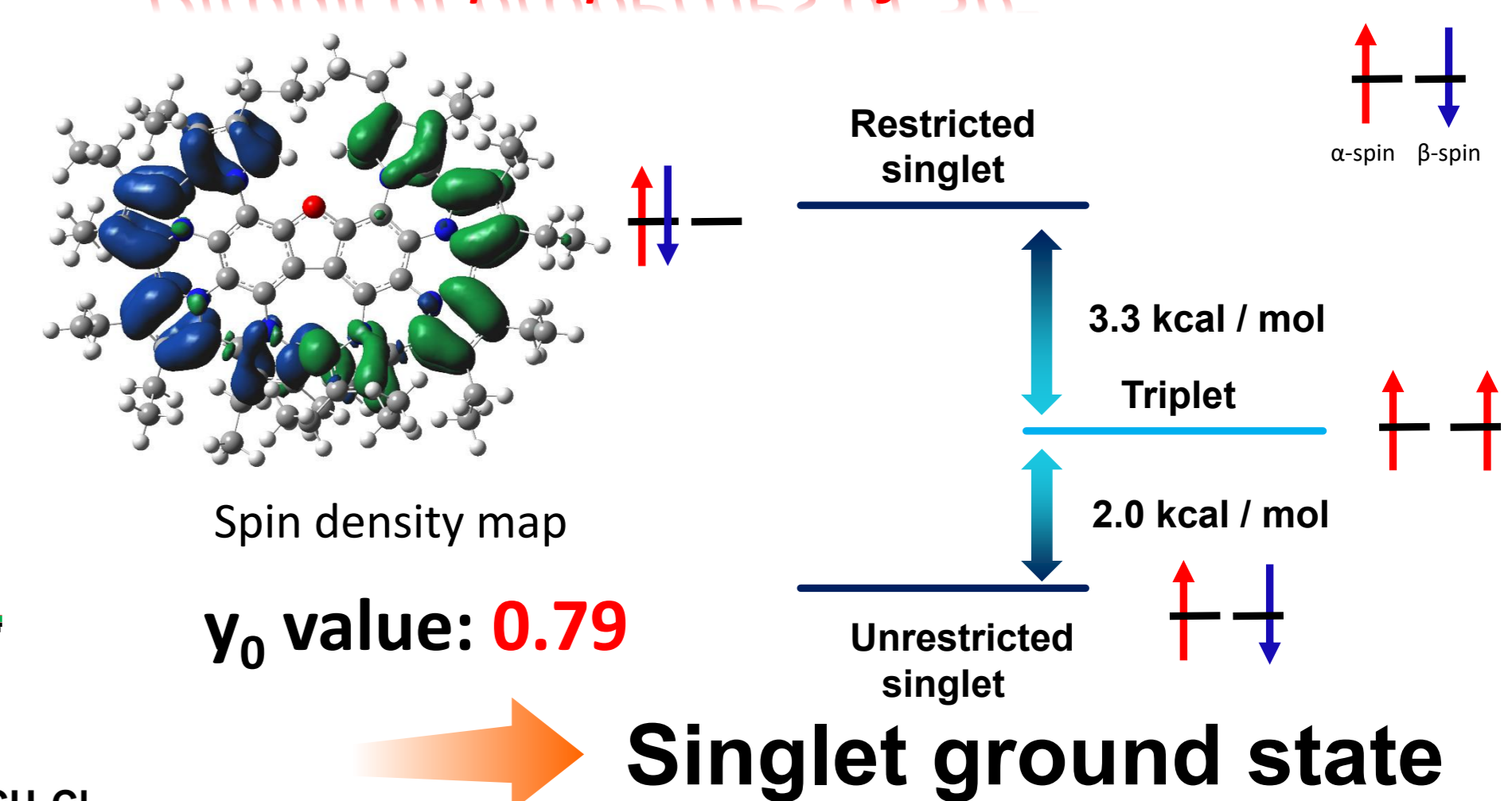
Stepwise oxidations of 3a



Spectroelectrochemistry of 3a



Diradical properties of 3b²⁺



Summary

- ◆ Compound 3a was synthesized via S_NAr reaction and Scholl reaction.
- ◆ CV and DPV measurements of 3a revealed four-step redox response.
- ◆ DFT calculations suggested that dication 3a²⁺ has a triplet ground state and 3b²⁺ has a singlet ground state.

