

Table S4 The orbitals contributing to S1~S5 excited states of Chl a/ β -Car aggregates.

	MO	Hole (%)	Electron(%)	Fragments	
				Porphyrin ring	Conjugated olefins
S ₁	388	78.724	—	√	
	390	—	87.957	√	
S ₂	389	71.277	—		√
	390	—	97.436	√	
S ₃	389	91.320	—		√
	391	—	91.182		√
S ₄	387	52.658	—	√	√
	390	—	78.529	√	
S ₅	388	73.980	—	√	
	391	—	60.202		√