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Probing the Role of the Eighth Bacteriochlorophyll in *holo*-Fenna-Matthews-Olson Complex by Simulated Two-Dimensional Electronic Spectroscopy SHU-HAO YEH, SABRE KAIS, Purdue University — The Fenna-Matthews-Olson (FMO) complex in green sulfur bacteria funnels the excitation energy from the outer antenna system to the reaction center. FMO is an important system for studying the excitonic energy transfer in biological system including photosynthesis. Recently crystallographic studies have confirmed the existence of an 'extra' bacteriochlorophyll (8-BChls), this additional BChl has been suggested to act as a linker to the baseplate. To investigate the role of this eighth BChl, we have simulated the two-dimensional electronic spectrum of the *holo*-form (8 BChls) of the FMO complex and compared it to its *apo*-form (7-BChls). Due to the comparable energy scale of the transition dipole coupling and the bath reorganization energy we have applied the hierarchy equation of motion (HEOM) to calculate the third order optical response functions, which are the crucial components to simulate the two-dimensional electronic spectra. Our simulated spectra show good agreement with previously published experimental studies; we have extracted dynamic details for the determination of energy transfer pathway in both forms.

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