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Operator-based exciton–vibrational (OBEV) modelling of *Rhodobacter sphaeroides* bacterial reaction centre using mean-field and one-quantum closures

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Bacterial reaction centres (BRC) exhibit strongly coupled electronic excitations embedded in a structured vibrational environment, where exciton delocalisation, vibronic fluctuations, and relaxation jointly shape optical observables. To connect microscopic Hamiltonian models with measurable spectra while retaining explicit bath degrees of freedom, we implement a Heisenberg-picture operator-based formulation. The electronic subsystem is represented by excitonic projection operators, while the vibrational environment is modelled as independent harmonic oscillators linearly coupled to site populations. This operator framework naturally yields a hierarchy of coupled equations for electronic populations/coherences and mixed exciton–phonon correlators [1]. To obtain scalable and tractable dynamics for a complex multi-site BRC model, we implement two complementary closures of the OBEV hierarchy. In the mean-field approximation (MFA), mixed exciton–phonon correlators are factorized, yielding a self-consistent set of equations that captures bath-induced fluctuations and reorganization efficiently. In the one-quantum approximation (1QA), the leading mixed correlators are propagated explicitly, incorporating quantum corrections responsible for vibrational sidebands and asymmetric broadening beyond MFA. Temperature effects are included through thermal ensemble sampling of initial bath configurations, and spectra are obtained from the Fourier transform of the ensemble-averaged time-dependent polarization. We present BRC simulations highlighting how (i) MFA, (ii) pure 1QA, and (iii) hybrid MFA+1QA partitions across frequency windows affect lineshapes and vibronic features, and we discuss the parameter regimes in which quantum corrections are essential. This workflow provides an efficient route for spectroscopy-oriented modelling of *R. sphaeroides* BRC [2] and establishes a foundation for extensions to multidimensional signals and comparison with experiment.

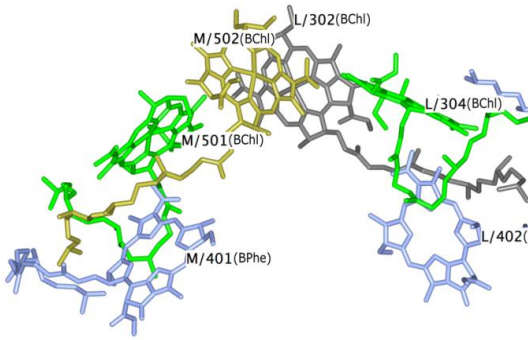

Fig. 1 The arrangement of the chlorophyll-type pigments of Rb. Sphaeroides. (PDB ID 2J8C).

REFERENCES

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