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A quantum dynamics descriptor for exploring a mechanism of light-driven electron migration in molecular aggregated system

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We introduce a practical calculation scheme for the description of excited electron dynamics in molecular aggregated systems by using a locally group diabatic Fock representation. This scheme makes it easy to analyze the interacting time-dependent excitations of local sites in complex systems.
In addition, this scheme can treat light-matter couplings, spin-orbit and non-adiabatic couplings. The present scheme is intended for investigations on the migration dynamics of excited electrons in light-energy conversion systems associated with photo-chemical functionalities.

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