Supporting Information: Simulating Non-Markovian Quantum Dynamics on NISQ Computers Using the Hierarchical Equations of Motion

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1 Quantum circuits

In this section, we give examples of the quantum circuits used in the main text. All quantum circuits were compiled according to the topology of the corresponding IBM quantum computer, specifically the IBM Sherbrooke, with the basis gate set consisting of X, $\sqrt{X}$, R_z, and ECR gates. The compilation processes were executed using the Qiskit package.[1]

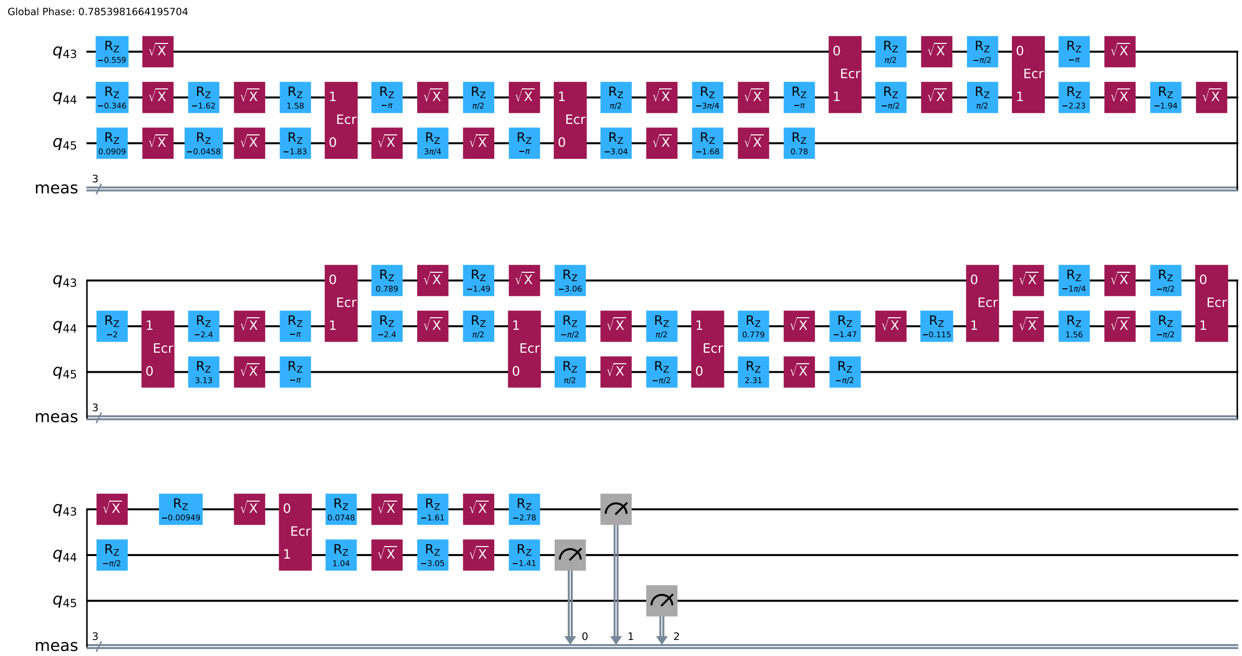

Figure S1: Quantum circuit for the molecular triad charge transfer model in the linear conformation, with the propagator at $t = 2073.5$ fs. The projection subspace $S = \{DD, DA, AD, AA\}$ corresponds to 3 qubits after dilation. The circuit depth is 60, with the following gate counts: 55 R_z gates, 38 $\sqrt{X}$ gates, and 11 ECR gates.

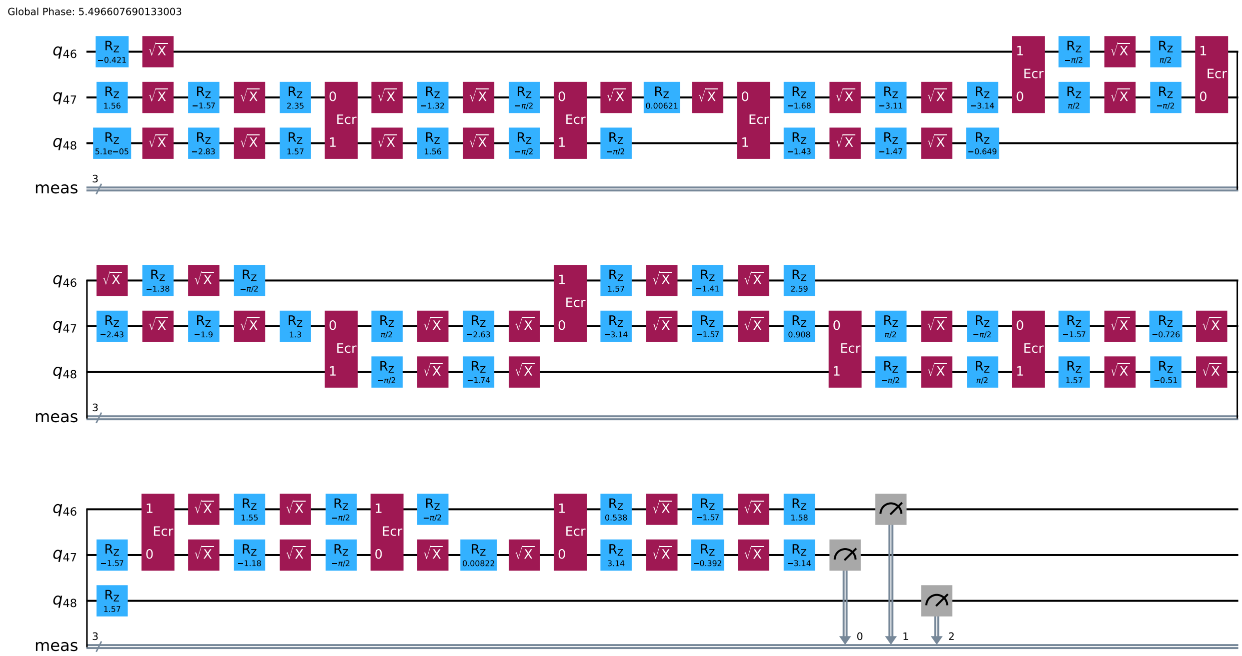

Figure S2: 3-qubit quantum circuit corresponding to the propagator at t = 612.0 fs for the excitation energy transfer model in the FMO complex, the projection subspace $S = \{11, 22, 33, 66\}$. The circuit depth is 67, with 60 R_z gates, 45 $\sqrt{X}$ gates, and 12 ECR gates.

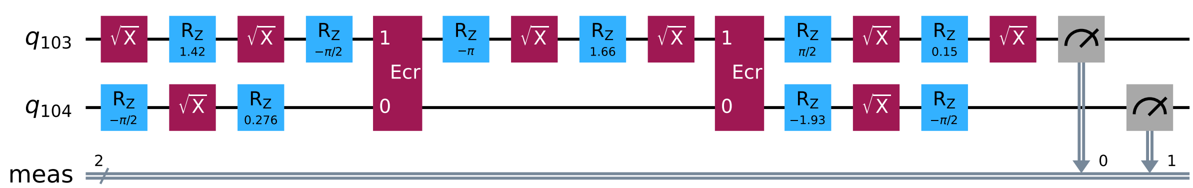

Figure S3: Quantum circuit for the 2-qubit linear conformation molecular triad charge transfer model (the projection subspace $S = \{DD, AA\}$), corresponding to the propagator at t = 2073.5 fs. The circuit depth is 15, with the following gate counts: 10 R_z gates, 8 $\sqrt{X}$ gates, and 2 ECR gates.

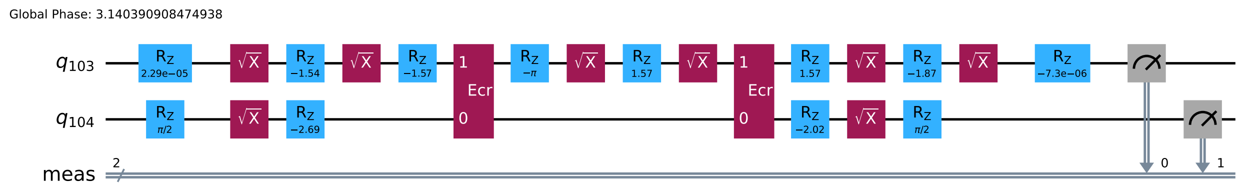

Figure S4: 2-qubit quantum circuit corresponding to the propagator at $t = 612.0$ fs for the excitation energy transfer model in the FMO complex, with the projection subspace $S = \{11, 22\}$. The circuit depth is 17, with 12 R_z gates, 8 $\sqrt{X}$ gates, and 2 ECR gates.

2 Results without error mitigation

This section presents the NISQ results without error mitigation techniques for charge transfer in the molecular triad and energy transfer in the FMO complex.

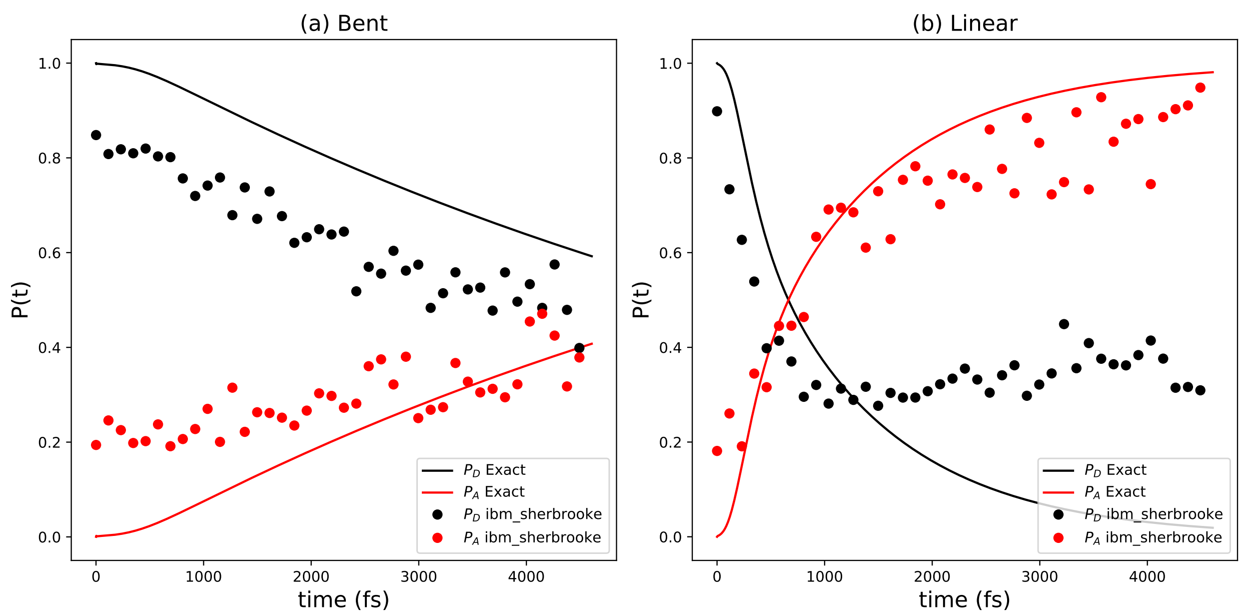

Figure S5: Population dynamics of the molecular triad without error mitigation: (a) Bent conformation, (b) linear conformation. P_D denotes the population in the $\pi\pi^*$ (donor) state, while P_A denotes the population in the CT1 (acceptor) state. The solid lines represent the exact HEOM results, and the scatter points represent the quantum circuit results from the IBM Sherbrooke computer. The projection subspace $S = \{DD, DA, AD, AA\}$. Each time point is measured at 20000 shots.

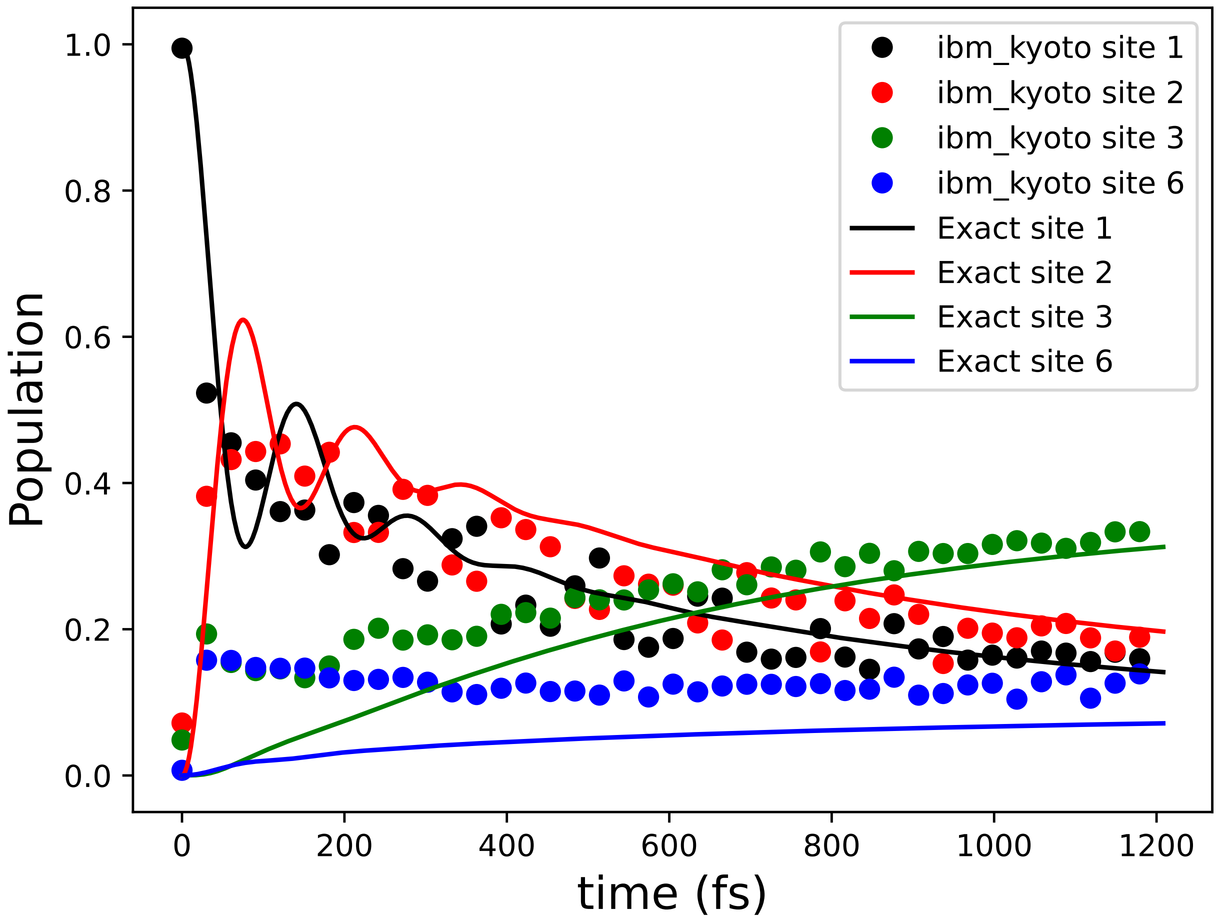

Figure S6: Population dynamics of the FMO complex without error mitigation. The solid lines represent the exact HEOM simulation results, and the scatter points represent the quantum circuit results from the IBM Kyoto quantum computer. The projection subspace $S = \{11, 22, 33, 66\}$. Each time point is measured at 20000 shots.

References

(1) Javadi-Abhari, A.; Treinish, M.; Krsulich, K.; Wood, C. J.; Lishman, J.; Gacon, J.; Martiel, S.; Nation, P. D.; Bishop, L. S.; Cross, A. W.; Johnson, B. R.; Gambetta, J. M. Quantum computing with Qiskit. *arXiv:2405.08810* **2024**,