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Design of Molecular Cluster Dynamics through Digital Quantum Simulation on a Trapped Ion Quantum Computer

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Electronic excitation of molecular clusters are the microscopic dynamics governing the efficacy of both photovoltaic cells and photosynthetic reaction centers, as well as those emerging technologies that lie in between. In most cases, accurately capturing the behavior of such systems requires understanding not only the electronic excitations, but also the dynamics of the vibrational degrees of freedom, to which they are coupled. Simulating the dynamics of such an expansive Hilbert space is a prime application of quantum computers. In this work, we experimentally simulate the transfer of an electronic excitation along a chain of macromolecules under a variety of conditions using a trapped-ion-based quantum computer. Our approach begins by using the relatively accessible spectroscopic data of an isolated macromolecule, pseudoisocyanine, as the input to a hybrid quantum-classical optimization algorithm which creates a digitally prepared wavefunction describing that macromolecule. Thereafter, we use an ab initio model to track the dynamics of a cluster of three macromolecules. We perform these simulations for a variety of different inter-molecular couplings by varying the relative angle between the molecules in the cluster, providing proof of principle for ab-initio design of molecular clusters with tailored excitation transfer rates.

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