Simulating Chemical Dynamics on Noisy Quantum Computers

We present a framework for the digital-analog simulation of Hamiltonians with linear-vibronic coupling (LVC) on quantum computers, and apply it to electron transfer in organic donor-acceptor systems, which present a promising platform for efficient charge separation in organic photovoltaic devices. Our approach turns the noise intrinsic to quantum hardware into a resource to emulate vibrational relaxation. Using superconducting quantum processors, we simulate charge separation from an electron donating thiophene polymer along a one-dimensional chain of fullerene acceptor molecules on, reproducing non-Markovian dynamics and scaling the chain length up to 10 acceptor sites, an unprecedented scale for chemical dynamics on quantum computers. Our model of vibronic electron transfer offers a portable, application-oriented benchmark for simulating long-lived entangled states on NISQ computers.