Photonic simulations of molecular quantum dynamics

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Modelling the dynamics of quantum mechanical systems, including molecules, is generally intractable to classical computational techniques. Such computational overheads may be overcome by utilising quantum simulation techniques, in which a well-controlled quantum system is programmed to mimic the quantum behaviour of another. Recent progress in integrated photonics has seen the advent of high fidelity on-chip processing of photonic quantum information and fully programmable circuitry to establish devices that are universal for linear optics. Progress has also been made in the integration of photon sources and single photon detection, which together with high-speed and low-loss photonic switches, enable a versatile class of photonic quantum simulators. It is hoped that the demands on error correction for specialised quantum simulators could be much lower than those for universal digital quantum simulators. Here we discuss proof-of-principle experimental demonstrations of quantum photonics as a simulation platform for molecular quantum dynamical behaviour. Using the analogy of optical modes in miniaturised waveguides for vibrational modes and single photons for quantised vibrational excitations, we simulate the dynamics of molecular systems, including time evolution for a range of different molecules, evolution of multiple excitations, anharmonics, thermalisation, and demonstrate applications including machine learning algorithms that identify disassociation pathways.