QUBIC
The Australian Research Council Centre of Excellence in Quantum Biotechnology

Title

Institution	University of Melbourne / University of Queensland
Project details	Title: Quantum molecular dynamics on a quantum computer Project description: Simulating quantum systems is one of the key promises of quantum computers, yet most calculations demonstrated on present-day hardware focus on static properties such as ground-state energies. Molecular dynamics — how nuclei move as electrons redistribute — is a substantially harder target: it requires the quantum device to track a wave-function coherently in time and to yield nuclear coordinates that can be compared against classical simulation. Extracting these coordinates goes beyond reading off a number at the end of a circuit; it requires care in how the molecular Hamiltonian is mapped onto qubits, how the evolving state is measured, and how those measurements are converted back into a physically meaningful trajectory. Getting this mapping right is what determines whether a quantum simulation reproduces real molecular behaviour or merely produces random numbers. This project aims to build a working framework for running such dynamics simulations on digital quantum hardware, for a small molecular system where the results can be checked directly against classical benchmarks. Expected aims and outcomes: • Executable code to perform coherent quantum time-evolution of a small molecular system on a quantum computer or classical simulator. The program should sample the nuclear coordinates following the evolution of the system • Results of running the code on a classical simulator • Results of running the code on a quantum device (time permitting) • Outlook on how the method can be scaled to larger systems as quantum hardware improves
Who can apply	Experience with scientific programming (Python preferred) is expected. In addition, experience in one or both of the following is recommended but not required: • Quantum computing or quantum physics • Quantum chemistry
Contact / Project supervisors	Michael Jones (michjones@unimelb.edu.au) Jorge Campos (j.camposgonzalezangulo@uq.edu.au)