Cambridge Quantum Computing achieves groundbreaking results in Quantum Chemistry

CQC gets VQE "off the ground" and provides an efficient route towards simulating excited molecules using quantum computers

CAMBRIDGE, UK, Nov. 20, 2019 - Cambridge Quantum Computing ("CQC") today announced an important breakthrough in quantum chemistry that will enhance and accelerate the commercialisation of quantum computing in an essential area of human endeavour - the search for new materials in sectors such as energy and pharmaceuticals.

Accurately simulating how atoms and molecules behave when absorbing energy is essential in developing advanced materials, such as efficient solar panels. Quantum computers provide a route to highly accurate simulations of such processes that are beyond the reach of today's classical computers. Whilst quantum algorithms, such as the well-known Variational Quantum Eigensolver ("VQE"), are particularly adept at running on current quantum devices, VQE has, until now, been limited to simulating electrons in their lowest energy state, which is not useful for example, for modelling sunlight hitting a solar panel to excite an electron and generate electricity. To simulate such so-called "excited" states, one had to run a VQE calculation for the lowest energy state followed by other algorithms designed for excited states, which consumes valuable computational resources.

CQC's Cambridge based team led by scientists David Muñoz Ramo and Gabriel Greene-Diniz have released a scientific preprint paper which details a ground-breaking achievement that breaks a logjam in exactly the problems noted above. In a recent article "Calculation of excited states via symmetry constraints in the Variational Quantum Eigensolver", CQC has, for the first time, exhibited how it is possible to adapt the VQE algorithm to directly calculate excited states in particular molecules, bypassing the need to first calculate the lowest energy state. This improves the efficiency of excited state calculations for many molecules of industrial interest and is an important and critical first step in developing next generation materials. The

breakthrough will be applied by CQC with immediate effect through their unique enterprise software platform for quantum chemistry calculations "EUMEN".

Read the complete scientific paper here: https://arxiv.org/abs/1910.05168

About Cambridge Quantum Computing

Cambridge Quantum Computing (CQC) is a world-leading quantum computing software company with over 60 scientists including 35 PhD's across offices in Cambridge (UK), San Francisco, London and Tokyo. CQC builds tools for the commercialisation of quantum technologies that will have a profound global impact.

CQC combines expertise in quantum software, specifically a quantum development platform (t|ket⟩™), enterprise applications in the area of quantum chemistry (EUMEN), quantum machine learning (QML), quantum natural language processing (QNLP) and quantum augmented cybersecurity (IronBridge).

For more information about CQC, visit www.cambridgequantum.com