Materials for qubits: challenges of computer modelling for quantum technology

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Large-scale quantum computing requires extremely high precision qubits. This includes qubits that have long coherence times, can be accurately calibrated and are free from uncontrolled parameter drift. While superconducting qubits are one of the leading quantum computing technologies, they are still significant challenges in addressing these requirements for large-scale devices.

Equivalent constraints have been addressed in conventional semiconductor electronics, often with the help of advanced computer simulation tools. Yet for quantum technology, we are facing entirely new difficulties in terms of the scale and precision required for design and simulation. Significant progress has been made in terms of automated circuit design and qubit control. However the underlying materials science is proving to be relatively difficult to simulate with the precision required for quantum computing applications.

I will discuss what are some of the fundamental challenges in simulating materials for quantum technology, specifically those relevant to superconducting qubits. These include the difficulties of modelling defects in amorphous materials[1, 2, 3], the fabrication process for superconducting qubits[4] and the electric response of Josephson junctions[5]. In doing so I will also discuss our recent efforts in this area to develop proof-of-principle simulation methods for superconducting qubits.

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[5] M. Cyster et al. *Phys. Rev. Res.* 2 (1), 013110 (2020)