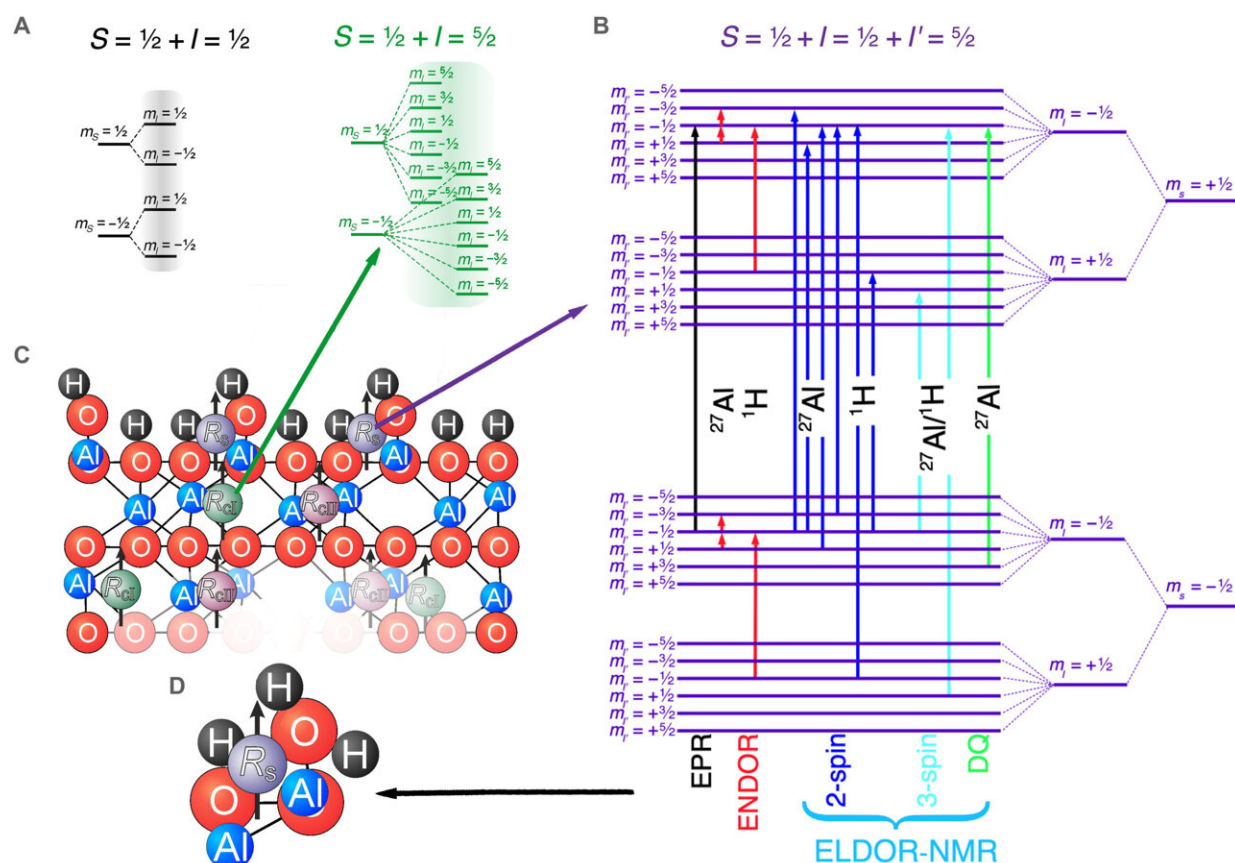# Advancing materials science for superconducting quantum circuits

April 27 2022

Identifying α-Al_2O_3 surface radicals by their proximity to proton nuclei. (A) The trivial energy levels of an electron spin (S = 1/2) coupled to a single proton (^{1}H, I = 1/2) and a single aluminum (^{27}Al, I = 5/2). (B) The combination of a proton and aluminum nuclei gives rise to a rich set of energy levels. Highlighted are the experimental techniques that we have used to map out these energy levels and reconstruct the environment of radicals. (C) EPR revealed three different radicals in α-Al_2O_3, here sketched near the surface of the Al_2O_3 crystal. The

NMR spectra of two of the radicals, R_{cI} and R_{cII} (green and rose spins), lacked multiple protons in their environment, locating them inside the crystal bulk. By contrast, the NMR spectra of a third radical, R_s, revealed a coupling to two structurally nonequivalent aluminum and at least three nonequivalent hydrogen atoms, meaning its only possible location would be near the surface. (D) Sketch of the deduced structure of R_s. Credit: *Science Advances* (2022). DOI: 10.1126/sciadv.abm6169

NPL scientists, in collaboration with experts in physical chemistry, have unleashed state-of-the-art electron paramagnetic resonance (EPR) techniques to understand materials relevant for superconducting quantum circuits, with results published in a recent paper in *Science Advances*.

Superconducting quantum computers have rapidly increased in size and complexity in recent years and the focus is now towards demonstrating fault-tolerant error-corrected quantum computing. Progress is currently held back by a relatively short coherence time and state fidelity of qubits. These obstacles are largely attributed to atomic-scale material defects interacting with the qubits. The origin of these defects is notoriously difficult to explore because of their quantum nature: They only reveal themselves at the energy scales and conditions relevant for the qubits themselves and are so far largely inaccessible by techniques available to material scientists.

By utilizing the inherent high resolution provided by high magnetic field EPR, in combination with nuclear spectroscopy techniques, the team were able to study a specific surface radical on Al_2O_3 (a material present in all modern superconducting quantum processors) in detail.

The study revealed a complex structure of the radical: an electron

coupling to multiple Al atoms in the Al_2O_3 lattice as well as many separate hydrogen nuclei. This in turn allowed to specifically attribute this radical to a surface defect. This is the first experimental work that is able to reveal the exact structure and insights into the formation chemistry of such surface defects that are linked to causing decoherence in superconducting quantum circuits.

Now, once we know the detailed properties of this defect, we can start to think about ways to silence it. Here silencing, as opposed to elimination, appears to be the most viable route for future devices with higher coherence, as this particular defect is now understood to be intrinsic to the chemistry naturally occurring at device surfaces.

The study presents an important advance in the field of materials for quantum circuits as it offers one of the first direct routes to chemical and structural identification of defects. So far, the field has relied heavily on materials science operating at entirely different energy scales and defect concentrations. These techniques can reveal imperfections but lack the ability to expose a direct link to defects that appear and interact with the quantum circuits themselves. We are therefore in urgent need for new materials science that can understand defects as and where they appear in quantum circuits without having to perform elaborate, and often inconclusive, correlation studies between materials, fabrication processes and device performance. The method presented in this study provides one of the first direct routes around this issue.

Sebastian de Graaf, senior research scientist, NPL said: "We are hopeful that our work will motivate material scientists and chemists around the world to apply and refine similar techniques to study the materials used in solid state quantum circuits. We can now, in a straight-forward way, investigate the impact of a wide range of chemical treatments with the goal of finding a process that reduces the amount of defects detected."

Provided by National Physical Laboratory