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Researchers simulate the design of new quantum bits for easier engineering of quantum computers

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Quantum computers—a possible future technology that would revolutionize computing by harnessing the bizarre properties of quantum bits, or qubits. Qubits are the quantum analogue to the classical computer bits "0" and "1." Engineering materials that can function as qubits is technically challenging. Using supercomputers, scientists from the University of Chicago and Argonne National Laboratory predicted possible new qubits built out of strained aluminum nitride. Moreover, the scientists showed that certain newly developed qubits in silicon carbide have unusually long lifetimes.

Quantum computers could break common cryptography techniques, search huge datasets, and simulate quantum systems in a fraction of the time it would take today's computers. However, engineers first need to harness the properties of quantum bits. Engineering new qubits with less difficult methods could lower one of the significant barriers to scaling quantum computers from small prototypes into larger-scale technologies.

One of the leading methods for creating qubits involves exploiting specific structural atomic defects in diamonds. Using diamonds is both technically challenging and expensive. Now researchers from the University of Chicago and Argonne National Laboratory have suggested an analogous defect in aluminum nitride, which could reduce the difficulty and ultimate cost of manufacturing materials for quantum computing applications.

Using the Edison and Mira supercomputers at DOE's National Energy Research Scientific Computing Center and Argonne National Laboratory respectively, the researchers found that by applying strain to aluminum nitride, they can create structural defects in the material that may be harnessed as qubits similar to those seen in diamonds. They performed their calculations using different levels of theory and the Quantum Espresso and WEST codes, the latter developed at the University of Chicago.

The codes allowed them to accurately predict the position of the defect levels in the band-gap of semiconductors. The researchers also closely collaborated with experimentalists to understand and improve the performance of qubits in industrial materials. Recently, they showed that newly developed qubits in silicon carbide have much longer coherence times than that of the more well-established defect qubits in diamond. Their results pointed to industrially important polyatomic crystals as promising hosts for coherent qubits for scalable quantum devices.

More information: Hosung Seo et al. Design of defect spins in piezoelectric aluminum nitride for solid-state hybrid quantum technologies, *Scientific Reports* (2016). DOI: 10.1038/srep20803

Hosung Seo et al. Quantum decoherence dynamics of divacancy spins in silicon carbide, *Nature Communications* (2016). DOI: 10.1038/ncomms12935

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