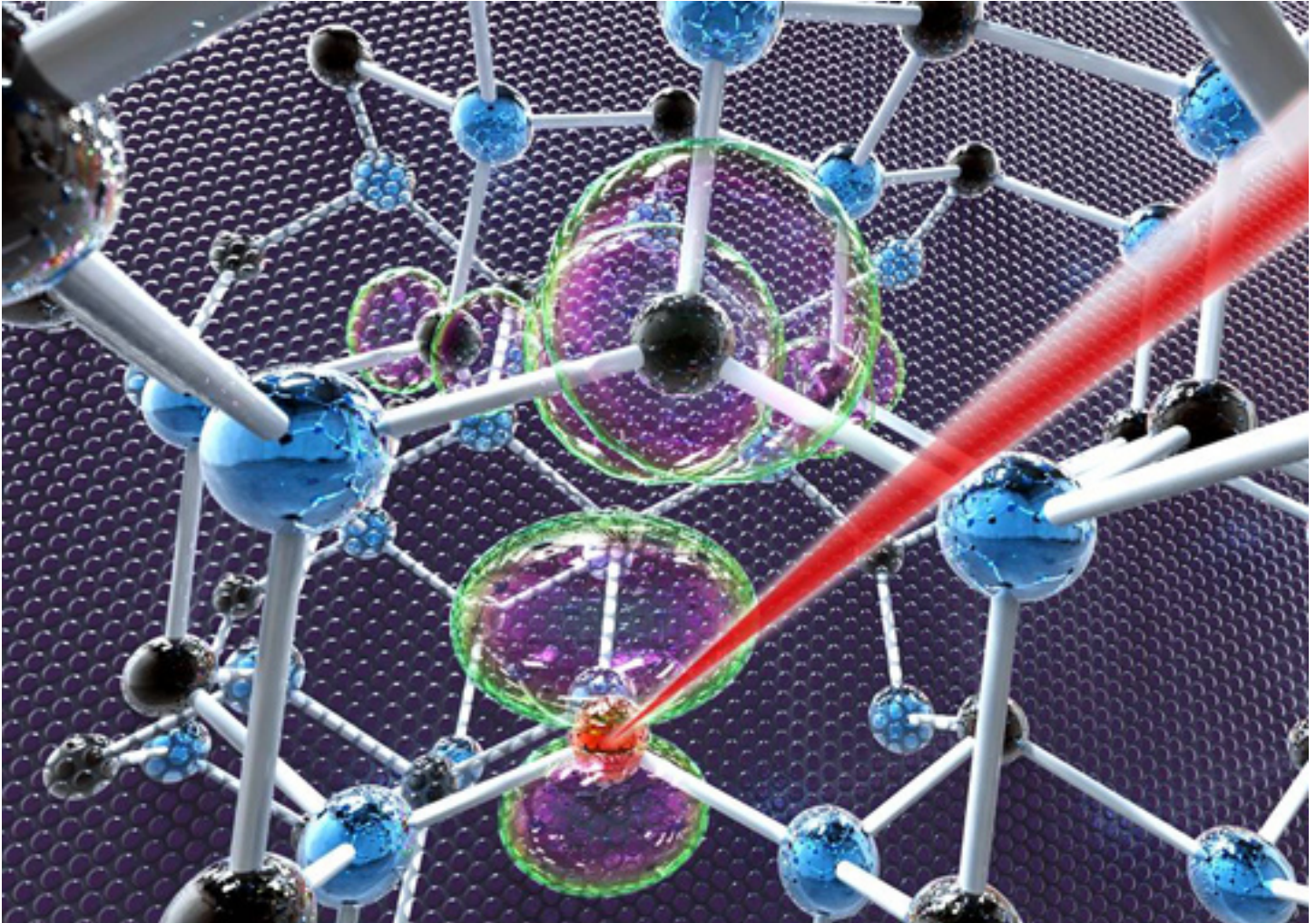


# Effective Defects

University of California researchers explore defects in diamonds and other materials useful for quantum computing



Artist's rendering of a defect in silicon carbide that is predicted to be a good qubit for quantum computing. The defect consists of a vacant silicon site and an adjacent substitutional nitrogen atom, and exhibits quantum properties similar to those of the well-known nitrogen-vacancy (NV) center in diamond. As shown, the quantum state of the defect is being probed by a laser tuned to an optical transition energy calculated for the defect. Image courtesy of J. R. Weber et al., and rendered by Peter Allen.

Quantum computers may represent the next major evolution in technology. In theory, they would allow for faster and more complex computations using a fraction of the energy. However, in practice, building a quantum computer remains a very tricky engineering problem from the atomic-level up.

At the atomic level, particles behave differently than they do in classical physics. According to the Heisenberg uncertainty principle, it is impossible to precisely determine the speed and location of a particle at any given moment. Instead, particles are characterized by a wave function that represents a probability that

the particle will be in a given state.

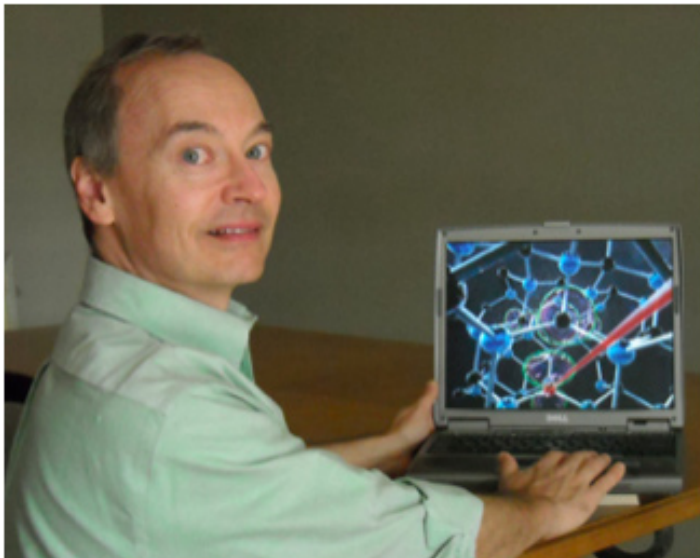
In quantum computing, instead of 0s and 1s, information can be encoded in the wave function and the infinite variations that are possible in the spectrum of the wave.

“You have a lot more flexibility in setting the values of the things that you compute,” said Chris Van de Walle, a professor in the Materials Department at the University of California, Santa Barbara, studying potential quantum systems. “You could basically have any continuous value that is being encoded in the wave

function of some entity that you are now using as your fundamental unit of computing.”

If it sounds far out, it is. Over the last decade, researchers have investigated various ways of designing a practical implementation of a quantum bit (or qubit) and none are near completion.

“If you can come up with such qubits and incorporate them in the computing architecture, it has been shown theoretically that you can solve problems computationally that are currently simply not feasible,” Van de Walle said. “The big challenge of course is to come up with specific implementations of these qubits.”



Professor Chris Van de Walle with an image of the defect in silicon carbide that is predicted to have applications in quantum information science. Photo credit N. Greenleaves.

### Promising Results from Diamonds

One of the most promising implementations involves not a thing, but an absence: a defect in diamond that leads to a missing carbon in the material's matrix, with a rogue nitrogen atom located nearby. This altered structure creates a hole, or vacancy, called an NV (nitrogen vacancy) center, with a specific wave function that many believe can be effectively manipulated for quantum computing.

In industry, defects are typically considered something to be avoided at all costs. However, in the case of materials for quantum computing, it is the defect that makes computation possible.

"For the quantum computing application, the defect is actually a good actor," Van de Walle said. "It's the qubit that you want to use as your unit of computation."

The biggest advantage of NV centers in diamonds is their ability to operate at room temperature, rather than requiring near absolute zero temperatures, as other quantum computing systems do. Also, electrons in the NV center can remain coherent for a long time and can be manipulated by outside forces.

"You can control where the vacancy is formed in the crystal and you can also probe it very accurately with laser beams with a specific wave length," he explained.

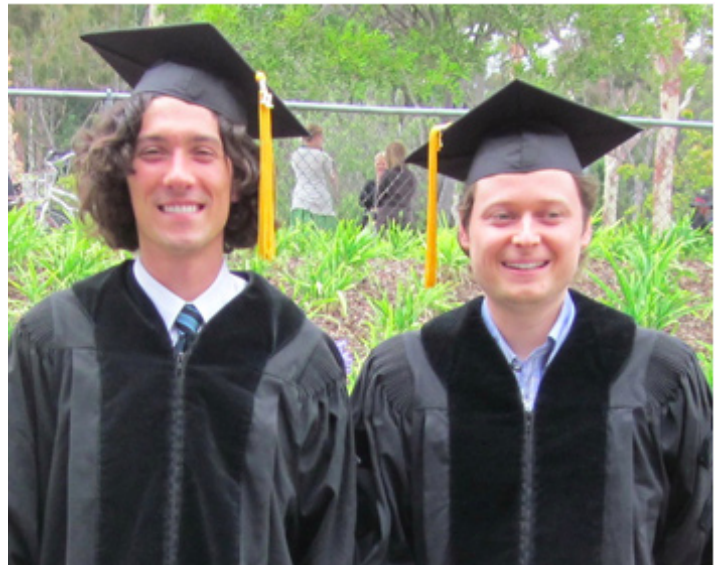
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Van de Walle, an expert in defects and impurities, has been working closely with David Awschalom, an experimentalist at UCSB and a leading quantum computing expert, to expose the atomic-level dynamics of the diamond center. Van de Walle's computational simulations on the Ranger supercomputer at the Texas Advanced Computing Center were able to match experimental results for the NV center.

They also added a few crucial pieces of information to the corpus of knowledge about the NV defect. In particular, they found that the charge state of the defect plays a crucial role in achieving a useable wavelength. This means controlling the number of electrons that can enter the vacancy by suitable doping of the material.

"For NV centers in diamonds, the optimal charge state is a -1 charge state," Van de Walle said. "For defects in other materials, it may be a different charge state, and just by guessing the charge state, you wouldn't be able to know if it's a good choice. But that's what we can calculate."



Joel Varley and Justin Weber, who performed the computational research on defect centers for quantum computing in the Van de Walle group, recently graduated with a Ph.D. in Physics from the University of California, Santa Barbara. Photo credit C. Van de Walle.

### Beyond Diamonds

There is one obvious problem with the NV center implementation. Diamonds are expensive and difficult to work with. To make a practicable system that could replace digital, silicon-based chips, the researchers needed a material with the same characteristics, but that was more common and easier to manipulate.

They used their earlier simulations as the basis for a set of criteria on what might make a useable quantum environment, and then started testing likely candidates. Most recently, Van de Walle simulated the behavior of silicon carbide (SiC). Like diamonds, silicon carbide can be prepared so that four carbon atoms surround a vacancy where a silicon atom has been removed. Single nitrogen atoms, too, can be placed in the appropriate location through ion implantation.

"That really looked to us like the closest similarity we could have for any defect in a material other than diamond," Van de Walle said. "Fortunately, silicon carbide is a lot cheaper, a lot more readily available, and a lot easier to process than diamond is, so it already meets a lot of the criteria that we are setting for the material to find a suitable qubit."

The researchers found that the properties of the silicon carbide center are in many ways similar to the NV center in diamond and hence suitable for qubits. In fact, in one way, the silicon carbide center might even be better than the center in diamond because its excitation energy corresponds to a laser wavelength that is closer to commercially available, cheap lasers.

The results of their research were published in the May 2010 edition of the Publication of the National Academy of Science.

To calculate the quantum mechanical interactions of hundreds of atoms requires thousands of computer processors working in tandem for days. "Without the ability to run on TACC's supercomputers, we would simply not have been able to do this project."

The high-fidelity quantum simulations are inspiring confidence among their experimental collaborators, and generating new ideas for lab experiments.

"The ability to take our expertise in the area of defects, and to use it creatively to design defects with certain properties is really great," Van de Walle said. "It's exciting to be able to dig into what we know about defects and use all of that knowledge to construct a defect with a given property."

It just goes to show that sometimes perfection is overrated.

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