Newcastle University

Making Computers out of Diamond:

An Exploration into Colour Centres as Quantum Bits

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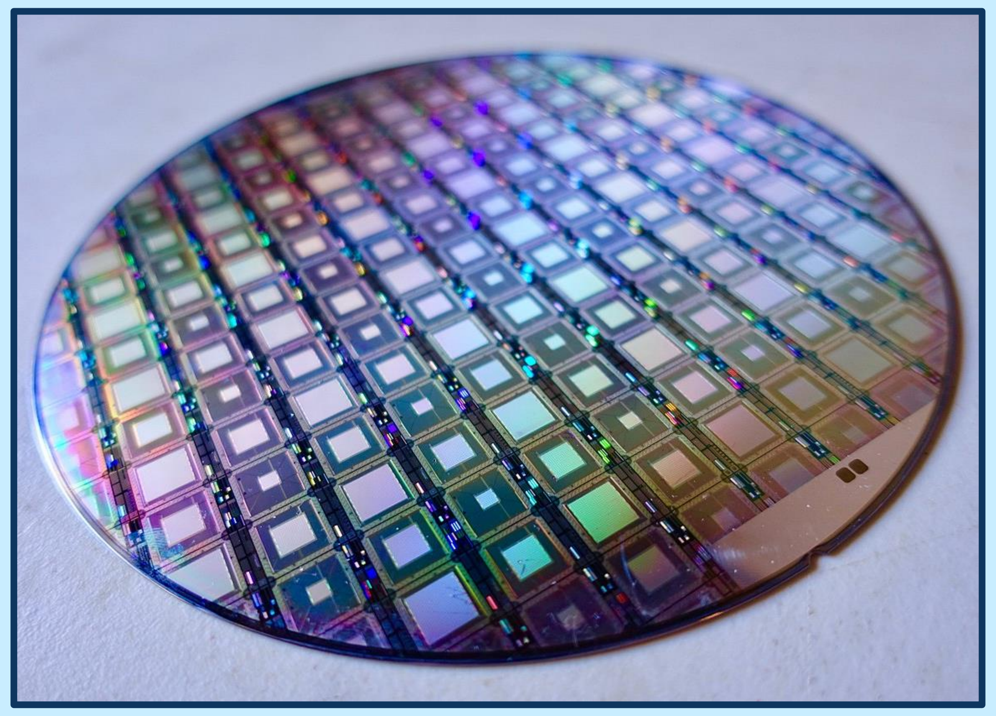
Introduction

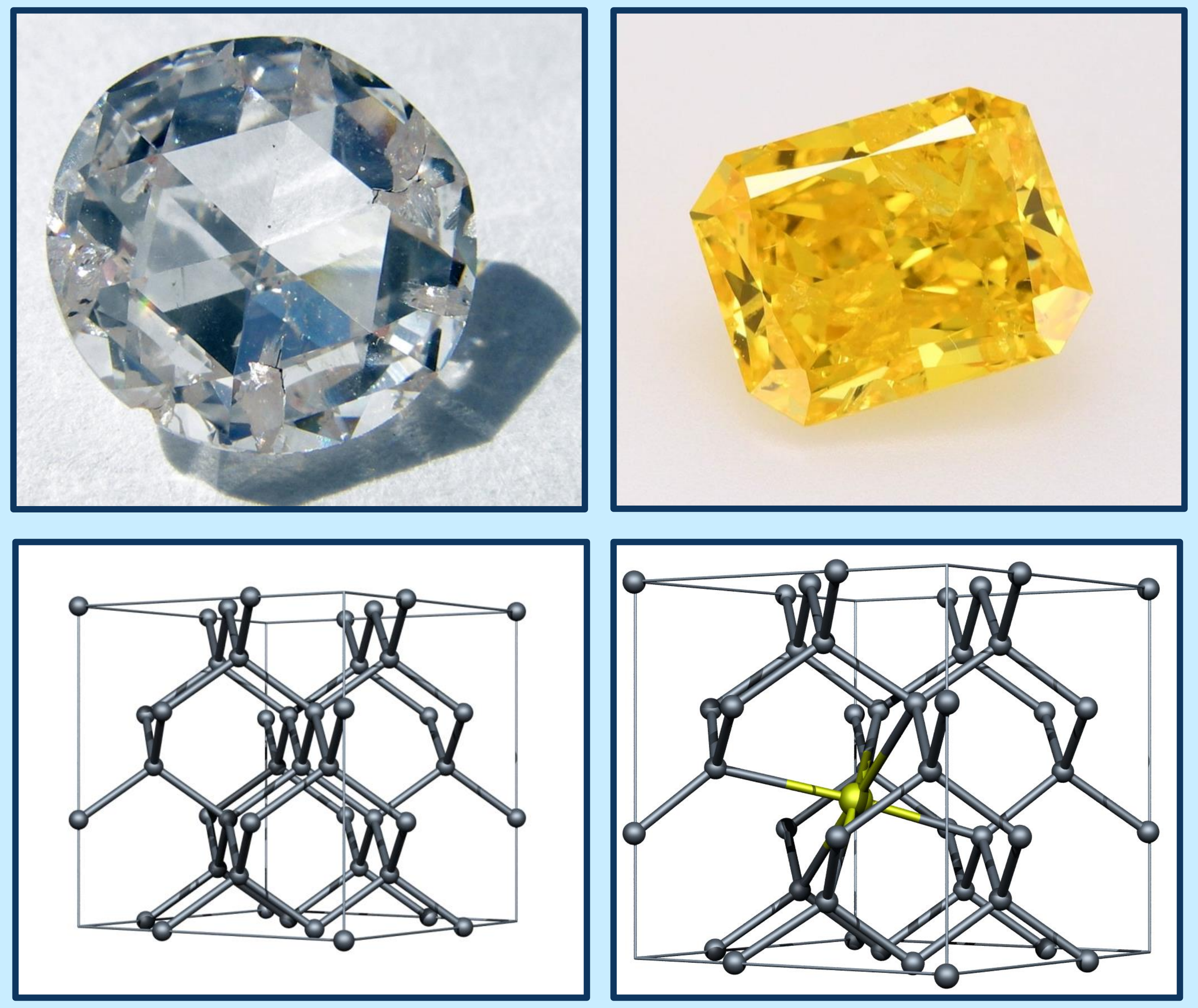
- Quantum Computing has proved to have far-reaching potential in many applications, from cybersecurity to "big data" problems
- The technology can solve problems in only a fraction of a second that might take a conventional computer billions of years

- A quantum computer is comprised of quantum bits (**qubits**)
- These qubits need a physical support to exist, like how a bit in a conventional computer needs a transistor
- Defects called **colour centres** in diamond can act as this physical support



What are Colour Centres?

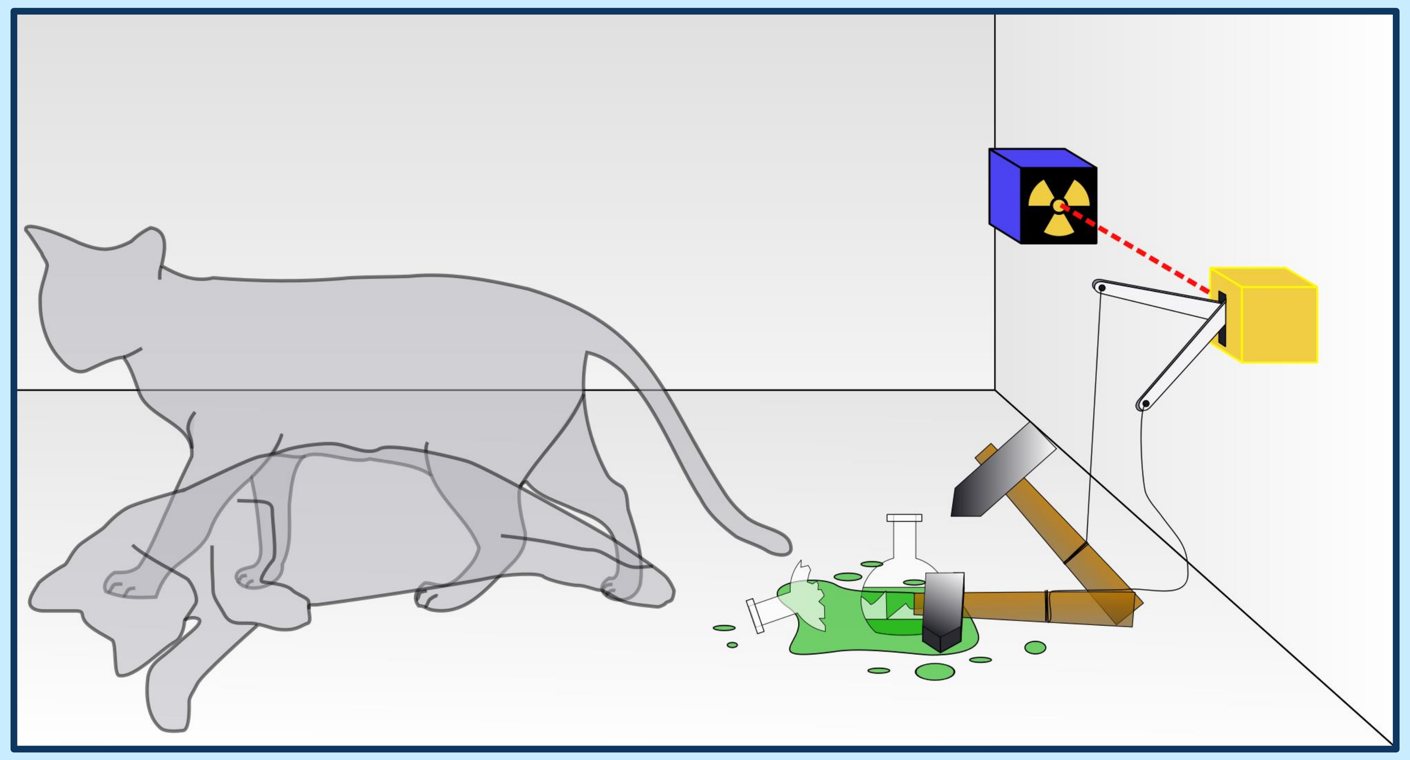
- A colour centre is a defect in the structure of a crystal that interacts with light and is therefore **optically active**
- A defect of only one atom in a thousand is enough to visibly change the colour, but for our purposes we may use an even lower concentration
- The defects we are using change the energy state of their electrons by absorbing certain colours of light
- By firing individual particles of light (**photons**) at these colour centres, we can detect what state they are in, and manipulate that state as well
- This idea is the basis of our Quantum Bit



Above, we can see the structure of diamond at the atomic scale, one pure and one with a colour centre implanted. Above these atomic diagrams are how photographs of how they look to our naked eye.

What are Quantum Bits?

- A conventional computer, like the one on your desk at home, represents its information as bits
- These bits can be in a state of either a 1 or a 0 (on or off)
- Similarly, a quantum computer represents its information as quantum bits (qubits)
- Unlike bits, qubits can be in a **superposition** of being both 1 and 0 (on and off) at the same time
- Qubits can also be **entangled**, meaning that the state of one qubit can instantaneously affect the state of another, even over arbitrarily long distances
- A quantum computer is comprised of many qubits working in tandem



- The concept of superposition is famously explored in the Schrödinger's Cat thought experiment (illustrated above)
- In it, a cat is placed in a box with a device that has some probability of killing the cat in a given time
- The idea is that until you open the box, the cat is in a superposition of being both alive and dead simultaneously
- This is analogous to how qubits work, with alive and dead being an analogue for 1 and 0

Aims and Method

The aim of this research is to study the behaviour of various impurities in diamond as colour centres, and to suggest potentially suitable alternatives to the already heavily studied Nitrogen-Vacancy (NV-) Centre.

This research will utilise Newcastle University's in-house quantum mechanical modelling software "AIMPRO" via the "Topsy" High-Performance Computing system to simulate the behaviour of various impurities in diamond. results can be used to develop the foundational information required to determine if a colour centre is viable.

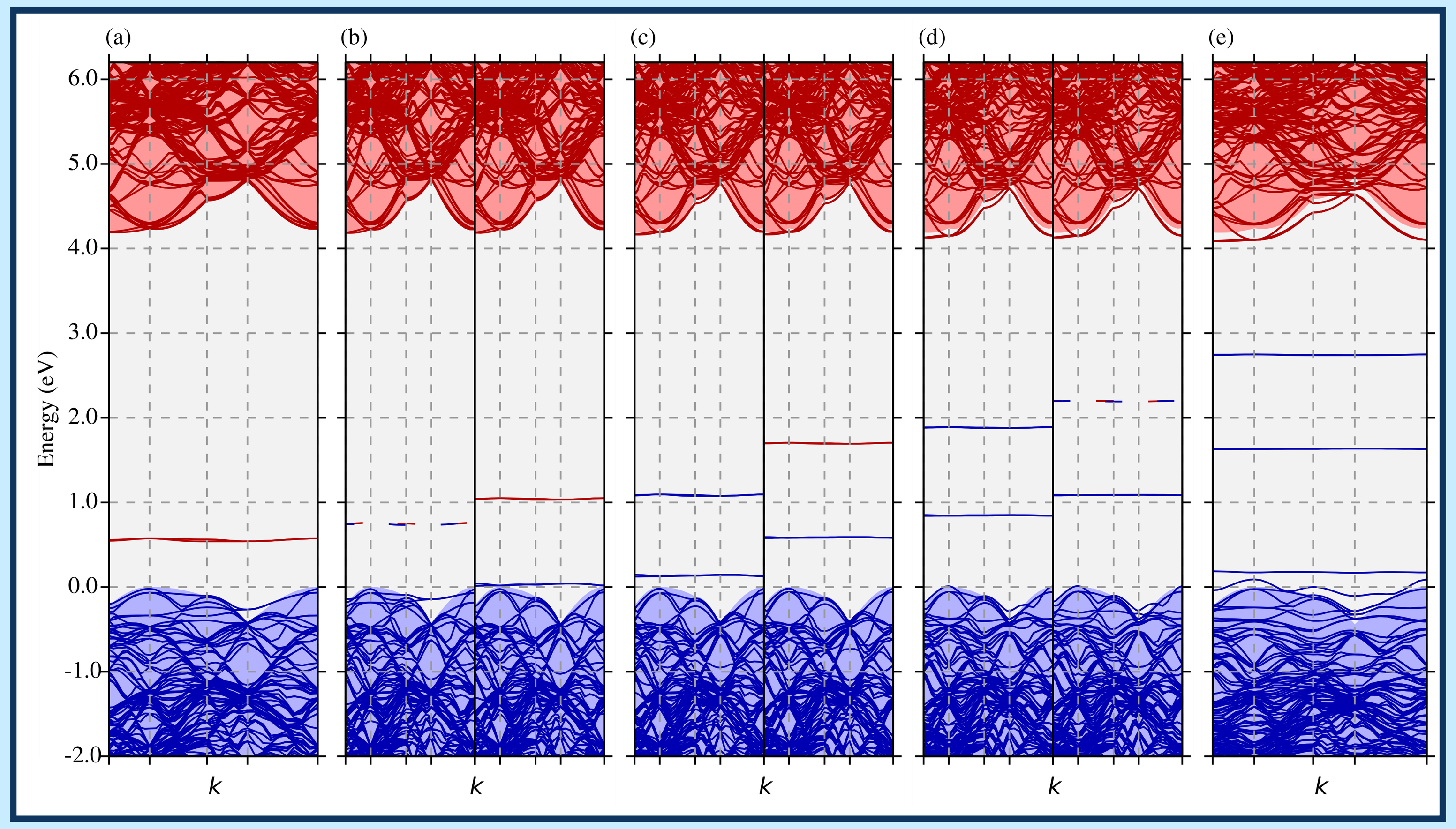
What Colour Centres Work as Quantum Bits and Why?

There are several criteria that a colour centre must meet to be a viable qubit. For each colour centre, the questions to ask are:

1. Can the colour centre form stably in real life?
2. Can its energy states be determined reliably?
3. Can its energy states be manipulated optically?

$$\Delta E = E_{TOT}(VA) - E_{TOT}(V) - E_{TOT}(A_s) + \mu_e$$

- Question 1 can be answered by a simple equation (shown above)
- Using it, one can determine if the energy of the structure existing is less than its components existing independently
- The universe prefers the structure of lowest energy to exist



- The above diagram (called a **band structure**) can help to answer questions 2 and 3. This example is plotted for different charges of Aluminium-Vacancy Centres in diamond
- It represents the occupied (blue) and unoccupied (red) energy states the electrons can have in the colour centre
- To be viable, a combination of occupied and unoccupied states is needed in the section of empty space (called the **band gap**)
- The energy between the red and blue lines in the band gap will tell us what colour of light can manipulate the energy states

Acknowledgements and Sources

Schrodinger's Cat diagram by Wikimedia user Dhatfield
Photograph of wafers by Steve Jurvetson
Photograph of Quantum Computer by IBM (all via CC)

Sources:
https://journals.aps.org/prb/abstract/10.1103/PhysRevB.105.165201
https://www.degruyter.com/document/doi/10.1515/nanoph-2019-0154/html

Conclusion

The simulations were able to model to a reasonable degree of accuracy the known properties of pure diamond and the Nitrogen-Vacancy (NV-) Centre, which gives credence to their modelling of the colour centres for which the properties are unknown.

These simulations showed that Aluminium (AlV-) may be a potentially viable colour centre and concurred with previous ab-initio modelling that Boron (BV-) may also be viable.