Quantum Mechanics *hidden in* Gems

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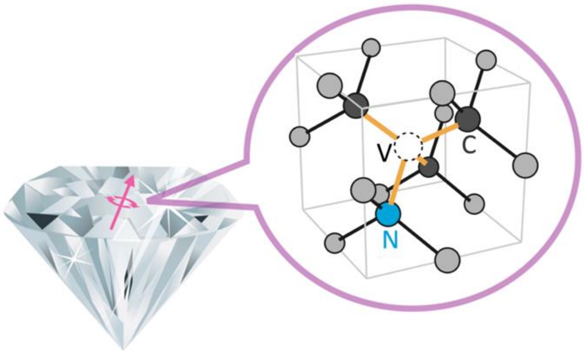
Sapphire, Diamond, Spinel, Quartz, etc., are all gems. What accounts for the beauty of these gems, especially their transparency and coloration? — Hidden beneath these properties lies quantum mechanics.



In these visual characteristics, particles called electrons play a significant role. Electrons are trapped in a lattice in any crystal and have a specific energy that can be transferred in-and-out through light emission/absorption. This property is therefore manifested in the appearance of matter. In some crystals, electrons are not allowed to take a specific magnitude of energy (Energy Gap). Matters with a larger energy gap are less likely to exchange light and become transparent.

Furthermore, skipping values of energy, like stairs, are sometimes possible in the energy gap. Such energy levels are given by defects of the host crystal lattice, i.e., impurities and vacancies, allowing electrons to emit light with specific colors. Those defects are the colorant of host materials and thus named color centers. A substance with a larger energy gap (transparency) and an ensemble of color centers (coloration) is the true nature of gemstones. For example, ruby is a wide-gap material called aluminum oxide, which acquires its red color from chromium-related defects.

Recently, color centers have attracted keen attention among researchers of quantum mechanics. Why would beautiful defects attract their attention? The short answer is that some of these color centers can be used as a readable and controllable "Qubit," a basic unit of quantum information.

For a moment, let me talk about "Qubit" that dwells in the color center. I said that in the color center, the phenomenon of "luminescence" itself was a manifestation of quantum mechanics. Of course, this is merely an observation of the merged phenomena that some electrons have gained/lost certain energy. However, the story is totally different for electrons trapped in "color center" orbitals. The electrons living here have fixed energy and sense the surrounding magnetic field. By shaking the magnetic field with a high frequency (applying microwaves), the state of the electrons can be manipulated to create a superposition of discrete states. Now that we have access to the quantum operation of particular electrons, then how can we "read out" the quantum information? In fact, there is a specific color center that makes this possible with "light" in a tiny fraction, about one out of hundreds or more.

The most typical example is the nitrogen-vacancy (NV) center of a diamond. There, electrons have some energy levels that can be reached by green light apart from the region that microwaves can manipulate, and when they return from there to the stable lower level again, in most cases, they emit red light and fall directly back to their original state. For some states manipulated below (called the one-state), however, it is possible to go to a specific state (called the zero-state) without emitting red light through a complex process. From this property, the electron's quantum state can be converted into macroscopic information in the form of "luminescence brightness." This is how we read out the state and meanwhile initialize it, a technique known as Optically Detected Magnetic Resonance(ODMR).

Color centers capable of ODMRs are essential for studying quantum mechanics and for the probes for "quantum sensing" that enhance the response of magnetic fields through quantum manipulation. Quite recently, a color center called Boron-Vacancy has been discovered in an unusual gemstone (wide-gapped material) called hexagonal Boron Nitride(h-BN), which is the main topic of this essay.

What is the h-BN? h-BN is a chemical compound of boron and nitrogen atoms having a graphite-like layered sheet structure. The atoms within each layer of h-BN bond firmly, but the sheets are stacked weakly, and a thin layered h-BN (down to a single layer) can be peeled off even by scotch tape! In addition to this unique feature that allows easy pull-off and stick-on using tape, it possesses an exceptional insulation performance even a single layer. Thanks to this, h-BN is widely used as an "insulating seal" in the research industry for micro-scale devices. (Great insulation is due to the large energy gap, which is why I call h-BN a “gemstone.")

This article[2] reports for the first time the ODMR capability of Boron-Vacancy. The Boron-Vacancies' indicated performance is sufficient for using a magnetometer and a platform for quantum engineering, which is a huge discovery, but has attracted less attraction than other ODMR-capable color centers. It is so new that not many groups may have been able to get their hands on it.

Why is this defect so important? Here its two-dimensionality takes advantage. Color-centers' Qubits sell themselves as stable, but their nature of being caged in a crystalline lattice is a bottleneck. Proximity is crucial for applying both as a magnetometer and an interacting quantum system. If we use the color centers inside ordinary crystals, such as the NV center in diamond, we cannot get close to the target magnetized object on the order of Å. Furthermore, they can only interact with surrounding nuclei of Carbon, Nitrogen or NV in a diamond lattice. However, remember that h-BN can paste on any material like a sticker. This enables h-BN to get close (down to several angstroms) to the target materials. As a nano-magnetometer, h-BN would open up direct imaging of magnetization and the current distribution of two-dimensional materials with really high spatial resolution, which was so far hard for other probes. Besides, Boron-Vacancy may be capable of interacting with nuclei outside the h-BN. If so, we will have access to local measurements of nuclear spin resonance. More to the point, a two-dimensional arrayed Boron-Vacancies might be possible, realizing a two-dimensional interacting quantum system beyond the one-dimensional chain system[3]. No report of such an experimental system exists yet.

Only a few months ago, a group from the University of California, San Diego, reported the first application of h-BN to wide magnetic field imaging of 2D materials[3]. Looking out over the world, some groups have already started mining Boron-Vacancy as a gem. A gold rush may be just around the corner.

[1] J. E. Shigley and C. M. Breeding *Gems and Gemology* **49**, 2 (2013)

[2] Gottscholl, *et al. Nat. Mater.* **19,** 540–545 (2020)

[3] Pai Peng, *et al. Nat. Phys.* **17**, 444–447 (2021)

[4] Mengqi Huang, *et al.* arXiv:2112.13570