Quantum information processing in carbon

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Abstract
We outline the recent advances in carbon-based quantum computer technology. This includes nanotube based, fullerene based and Diamond based quantum computer technologies.

Introduction

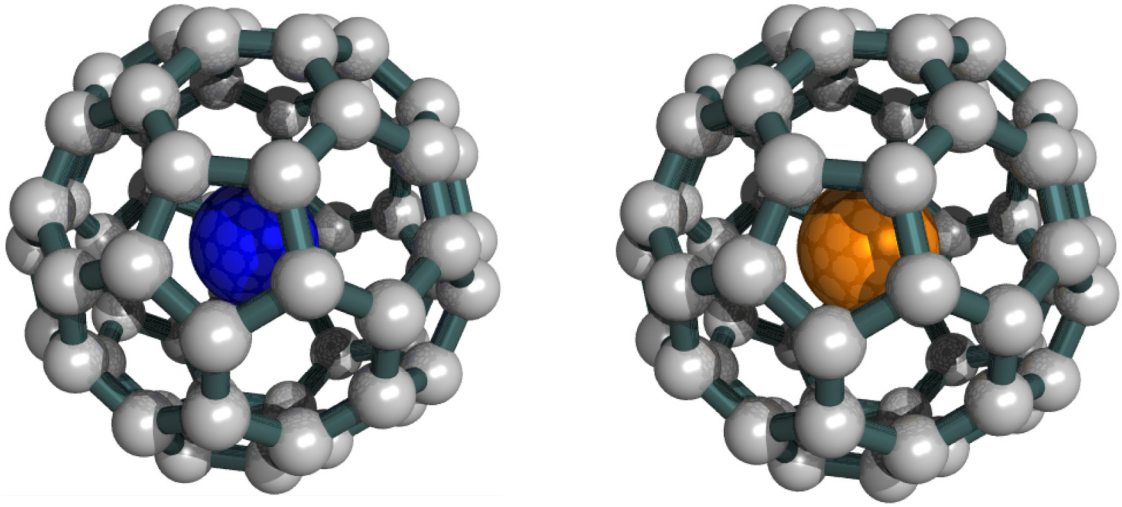
A room-temperature solid-state technology represents the "holy grail", in the search for a viable, scalable technology for quantum information processing (QIP). Until recently, achieving such a goal might have seemed "science fiction", but the recent achievements of a number of researchers (some FET funded and some non-FET funded), in the area of carbon-based QIP have prompted a serious rethink and indications are that this fledgling niche area of QIP research (carbon-based technologies), has the potential to exceed many expectations.

Solid-state QIP technologies are mostly based on existing technologies: superconducting circuits, quantum dots, semiconductor heterostructures, doped Silicon devices, etc. Of course, to achieve the technological advances required to perform QIP, such existent technologies need major developments and these are underway. These developments are aided by the (sometimes), enormous banks of knowledge that already exists with respect to these technologies and materials. One avenue of QIP research which does not benefit from such a preexistence of expertise but despite this, is making very rapid progress, i.e. the black-sheep of QIP technologies, are those technologies based on carbon. These carbon-based QIP proto-technologies include: nanotube materials where quantum spin-dots/qubit are located in the nanotube wall itself, nanotubes which enclose electron spin/qubit carrying molecules, individual fullerene (or Buckyball) molecules which are altered to encapsulate electron spin/qubits and finally bulk carbon (in the form of Diamond), which is engineered to contain electron spin/qubits within special defects of the Diamond lattice known as Nitrogen-Vacancy defects. In this article we will focus primarily on the last two of the above, the Buckyball molecules (C60), which have been altered to encapsulate a single Nitrogen or Phosphorous atom and the Nitrogen-Vacancy (NV), defect in Diamond.

Buckyball Qubits

Buckyballs are the common name given to a very special type of carbon molecule discovered in 1985 by Robert Curl, Harold Kroto and Richard Smalley Harry Kroto, who were awarded the Nobel Prize in chemistry for their work in 1996. The molecule contains sixty carbon atoms all connected together like a round soccer ball (**Figure 1/ Subfigures Figure 1a and Figure 1b**). In 1997, researchers at Berlin's Hahn-Meitner-Institute (HMI), accidentally discovered that Buckyballs could be formed around atomic Nitrogen and later on, around atomic Phosphorous [2] (shorthand N@C60 or P@C60). This interesting molecule was reported in the literature and preliminary investigations by Alois Weidinger and his colleagues at HMI into its structure indicated that it possessed unpaired electrons and that (most unusually), the Electron-Spin-Resonance signal indicated that the trapped Nitrogen atom was not interacting chemically with the sixty carbon atoms of the Buckyball cage. It appeared that this molecule was acting as a nanoscopic (diameter of 1nanometer), neutral atom trap for the Nitrogen atom! In 1999-2000, the European Future and Emerging Technologies programme launched it's proactive call for research into Quantum Information Processing and Communication and J. Twamley put forward the plan of examining these types of Buckyballs as potential elements in a quantum information processor. The research plan was ideally suited to the FET proactive programme, as although the basis for the ideas were sound enough, the research was high-risk, long-term and the research team was spread over many nations within the EC. This latter aspect was necessary as the expertise to tackle the question just did not exist in a single country. The research was funded by the FET and the two-year project [QIPDDF], produced valuable milestones such as the proposed use of the magnetic dipole interaction to coupled neighboring molecules [3], a quantum computer design using the material with individually addressed qubits [4], and a design without using individually addressed qubits [5]. The research also told us much more about this unusual

material which we will summarise below. Another vital element of performing research via European Union programmes is the ability to meet new colleagues and to form new and long-lasting research collaborations and the FET QIPC Conference meeting in 2001 in Torino, Itlay brought together many of the partners which make up a more recent FET project focused on developing a readout technique to determine the electronic spin state of a single N@C60 molecule. This project, QIPDDF-ROSES, has also produced a number of milestone discoveries such as the execution of a two-qubit gate in Diamond [5], improved synthesis techniques to yield 100% pure Buckyball materials, evidence that the NV-Diamond system can coupled to the Buckyballs via magnetic dipole interactions and the performance of detailed quantum control of the NV-Diamond system via the execution of Quantum Process Tomography. ***Without the FET programme, the "black sheep" concept of utilizing the trapped spin system within a Buckyball would not have been examined.*** The potential use of this system as evidenced by the results of the original FET project QIPDDF, has expanded and now this material is being studied by a number of other research consortia all over the world for use in quantum information processing and otherwise.



(a) (b)

Figure1: Schematic diagram of doped Buckyballs, (a) Nitrogen in C60 or N@C60 and, (b) Phosphorus in C60 or P@C60.

As a means of categorizing the current status of development of Buckyball mediated QIP let us follow roughly the first five DiVincenzo criteria for a physical implementation of QIP technology [6]. These are that one must: (DiV 1) have a well defined extendible qubit array, (DiV 2) be able to initialize the qubit array into a known state, e.g. the "00000…" state, (DiV 3) the quantum information must survive in this array for a long time compared to the duration needed to execute a quantum gate, i.e. long decoherence times ($>10^4$ gate operation times), (DiV4) be able to have enough control over the qubit array to execute the basic universal set of quantum computer operations, and finally (DiV 5), be able to read out the state of the qubit array at the end of the computation.

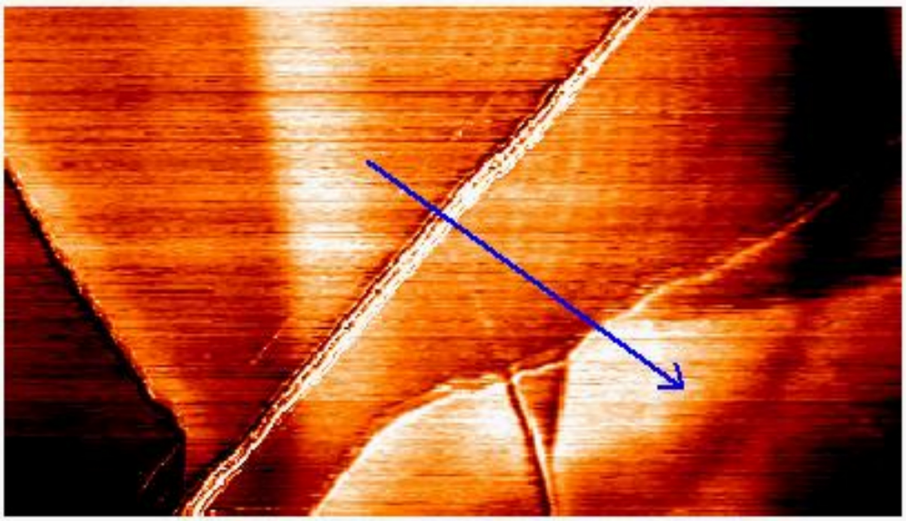


Figure 2: Scanning Tunneling Microscope (STM) image of rigid self-assembled Buckyball wire. Wire is several Buckyballs thick but can be rigidly pushed across the substrate in the arrow direction by the STM tip.

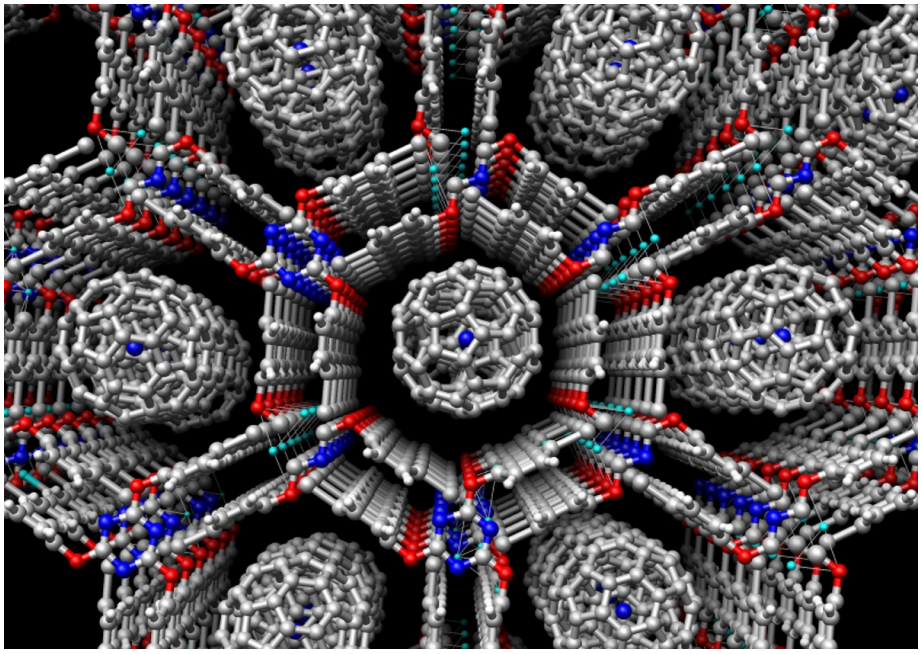


Figure 3: Schematic of experimentally self-assembled molecular tubes of doped Buckyballs.

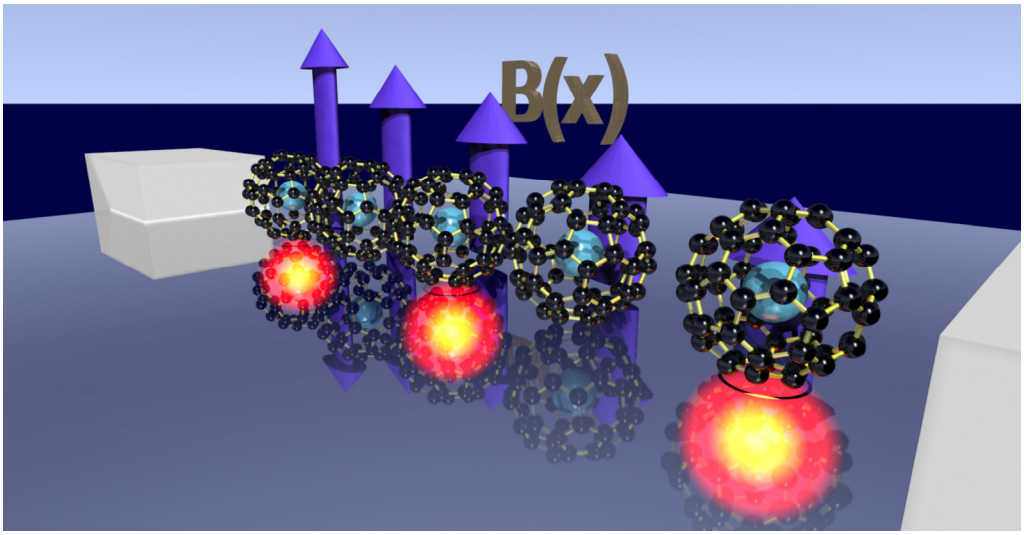


Figure 4: Schematic of theoretical Buckyball processor device consisting of a linear array of Buckyballs on Diamond between two current carrying wires with Nitrogen-Vacancy defects in the Diamond registered below specific Buckyballs in the array. The current though the wires creates a magnetic field gradient (B(x)), along the molecular array. The NV defects act as the optical inputs & outputs to the processor.

DiV 1 (*qubit array*): it is now possible to produce 100% pure Nitrogen or Phosphorous Buckyball material. We now know that each of these molecules contains a very well defined spin system and thus can contain a qubit. Thus the hard work of mechanically isolating an individual qubit has been done already via "chemical" means, one molecule = one qubit. We understand well that engineering via a top-down approach on nanoscale dimensions is incredibly tough but the use of carbon-based qubit materials allows fantastic bottom-up self-assembly chemical techniques to be used. This allows individual Buckyball wires to be fashioned (**Figure 2**), while huge numbers of parallel identical Buckyball wires can be fashioned quickly via self-assembly (**Figure 3**). One possible quantum processor design is shown in (**Figure 4**), and this will require the fabrication of a linear array of molecules, then registered with a few metal wires and buried NV readout systems.

DiV 2: (*initialize the qubit array):* Initializing these molecules to a known state will be possible once a readout system has been developed.

DiV 3: (*long decoherence time):* The trapped electron spin decoherence properties are, undisputedly, the single most astonishing property of these Buckyball materials. The dephasing time (or T_2), for the trapped Buckyball electrons has been measured to be at least 250microseconds, though this is at low temperature. This feature was already hinted at in the original Electron-Spin-Resonance experiments of [1], and this time may prove to actually be much longer as our measurements grow more sensitive. Theoretically, however, with such an enormously long lifetime for the trapped quantum information, we should be able to perform $\sim 10^4$ quantum gate operations, matching trapped ion quantum information processor designs. It is quite possible that these Buckyball materials possess the longest lived electron coherence times outside a crystal defect structure and although we have some insights as to why this is, the complete story regarding their long-lived electron states have yet to be fully understood.

DiV 4: (*execute quantum computer operations):* Two separate designs for a quantum processor have been developed. The first one [3], uses currents flowing thru small wires to

generate a large magnetic field gradient which will cause each of the spin systems in the molecules to possess different resonant frequencies. One can then apply microwave radiation pulses to the entire processor at the appropriate frequency to address a single specific molecule. Each molecule is separated from its neighbor by <10 nanometers and they interact via magnetic dipole coupling. The second design [4], uses an alternating array of P@C60-N@C60-P@C60… with no magnetic field gradient to perform quantum cellular automata quantum information processing. Here one addresses many molecules at once but by having two molecule types in the linear array one has enough flexibility to perform full blown quantum computation.

DiV 5: (*qubit readout*): This is the most challenging obstacle towards using these molecules as components in a solid-state quantum information processing device. No technology to-date can determine the spin-state of the electrons trapped within an individual Buckyball. Developing such a technology has been the sole focus of the recent FET QIPC project QIPDDF-ROSES. Among various possible candidates, buried Nitrogen-Vacancy defects in Diamond coupled magnetically to the Buckyballs have shown to be very possible. The NV-defect system will allow a fast ***optical readout and reset*** of quantum information stored in the Buckyball array. The quantum information will then be manipulated via microwave pulses. Towards this end we have studied the NV-defects themselves as we will have to be able to manipulate the readout systems with great precision. By making use of techniques from single molecule spectroscopy and optically detected magnetic resonance we have been able to find NV-defects with nearby ^{13}C atoms. We have then been able to execute a two-spin quantum gate coupling the electron spins of the NV-defect to the nuclear spin of the ^{13}C (see more below). Over the past year, though international collaborations, we have been developing NV-defect Diamond synthesis techniques that have produced ultra-pure samples. Such samples, like the Buckyballs, have extremely long decoherence times (>300 microseconds), but amazingly, at **room temperature.** Top-down techniques to implant NV-defects with nanometer resolution are under intense development but, as visualized in **Figure 4**, the spacing of NV-readout systems might not need to be so small and a combination of top-down fabrication of the NV-readouts coupled with bottom-up fabrication of the Buckyball linear array might do the trick. Most recently, we have achieved another milestone, only previously achieved by NMR QIP, all-optical QIP and trapped ion QIP where have been able to interrogate the quantum coherence properties of the NV-systems themselves using a procedure known as Quantum Process Tomography (Figure5_21).

In summary, through the opportunities made available for pro-active collaborations on a European level by the Future and Emerging Technologies Unit, Buckyball quantum processing technology has emerged from being a theoretical concept to being a worldwide research area which it rapidly achieving goals undreamed about previously.

Defects in Diamond: A Potential Hardware for Quantum Information Processing

Diamond is one of the most fascinating materials. As a gemstone, hard coating and future electronic material it is of economical relevance. Pure diamond is colorless and optically transparent. The most valuable gemstones are made from such material. Often however, diamond is coloured. In fact 80% of all stones found in nature are classified as colored diamond. A large number of impurities in diamond are so called color centers, which determine the color of the crystal. Famous examples are blue diamonds, where the color comes from trace amounts of boron. Most color centers are known in detail and are used

commercially to enhance the color of certain gemstones making them more valuable. Usually their chemically composition is simple, like a single impurity atom as in the case of the boron defect. Due to a substantial progress in material production nowadays diamond, which is practically free of impurities, can be synthesised. These developments together with the controlled generation and implantation of color centers have fostered the application of diamond in other areas of future information technology, namely QIP.

Recently different research groups in Europe have shown the potential usefulness of color centers in diamond as single photon sources for secure data transfer in quantum communication. Such single photon sources are novel type of light sources, which emit single photons on demands being a key element in quantum cryptography. Currently the most promising experimental approach uses single quantum systems as photon emitters. In this technology a single quantum system is excited by an external photon source or pumped electrically, the concomitant emission of a single photon is used to encode quantum information. A couple of quantum systems like ions, quantum dots, molecules or colour centers have been investigated. Figures of merit in the field are room temperature operation and high photostability of the system. Also, the photon emission rate should be high enough and the emission wavelength should be compatible with telecommunication requirements. Color centers in diamond meet most of these requirements. As an example, the nitrogen vacany defect center in diamond has been shown to be a stable room temperature single photon emitter. The advantage as compared to other sources is the unsurpassed photostability and ability to position single NV centers with high spatial accuracy. Narrow room temperature emission lines are found in Ni related defect centers in diamond. Production of synthetic diamond containing NV color centers has been shown. The defect is bright, emits at a wavelength where telecommunication fibers have low absorption and has a narrow room temperature emission wavelength. In the next couple of years it can be expected that an easy-to-use and robust single photon modules can be developed from single defect centers in diamond. The aim will be to develope a fiber-based compact module which will contain all necessary elements in a single piece of optical fiber. Such fiber modules might allow for transform limited single photon emission when operated at low temperature and hence might be an enabling technology for all optical quantum computing.

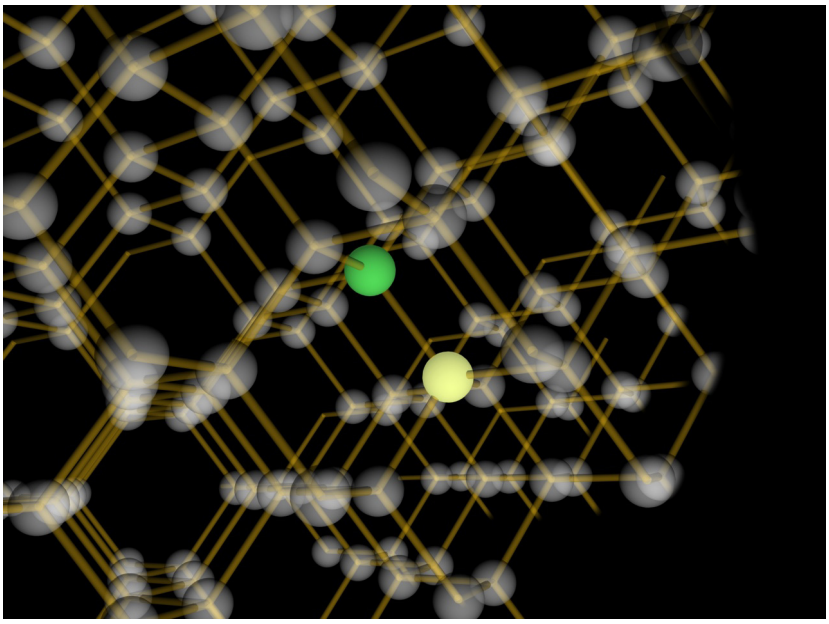


Figure 5: The nitrogen (green) and vacancy (yellow) forms nitrogen-vacancy defect in the diamond lattice.

A couple of defect centers in diamond are of potential use as quantum bits (qubits) for quantum computing as well. A prominent example is the nitrogen vacancy defect center (see **Figure 5**). In this defect the electron spin can be used as a quantum bit. It has been shown that the state of a single qubit can be read out at low temperature. Moreover, single and two-qubits manipulation is feasible even at room temperature [5, 7] (see **Figure 6)**. An important figure of merit is the dephasing time which is up to 0.35 ms under ambient conditions for this system. Qubit manipulations occurs on a timescale of some ten nanoseconds. Hence more than 10^4 qubit operations can be carried out before dephasing occurs. Nuclear spins are expected to show even longer dephasing times and hence are particularly interesting candidates as qubits or quantum memory. In the NV center nuclear spins are coupled to electron spins and hence are accessible as qubits as well. In this way quantum logic operation with a single electron and nuclear spin at a nitrogen vacancy defect center under ambient conditions have been demonstrated. In this scheme only nuclear spins which are sufficiently close (few 10^{-10}m) to the electron spin can be used. Hence this scheme cannot be scaled to larger number of qubits by adding nuclear spins. A scalable scheme requires the mutual coupling of defect centers. For this nitrogen atoms need to be implanted in diamond with high spatial accuracy. The precision needed is subject to the interaction chosen. For magnetic dipolar coupled centers, distances should not be larger than 5 nm, while for optical transition dipole coupling the distance can be as large as 10nm. Recently it was shown how to generate coupled defect center pairs by implantation of nitrogen molecules. In future devices advanced nano implantation techniques like the deposition of nitrogen atoms through moveable nano apertures need to be used. In these techniques low energy nitrogen ions (kinetic energy smaller 7keV) are implanted into a diamond substrate through a small (diameter 5nm) hole in the tip of a cantilever of an atomic force microscope. To allow for the addressing of single quantum bits, magnetic or electric field gradients need to be applied via gate electrodes. Owing to the close proximity of the defects, the requirements on the nanofabrication of the device are quite stringent though not beyond the capability of current technology.

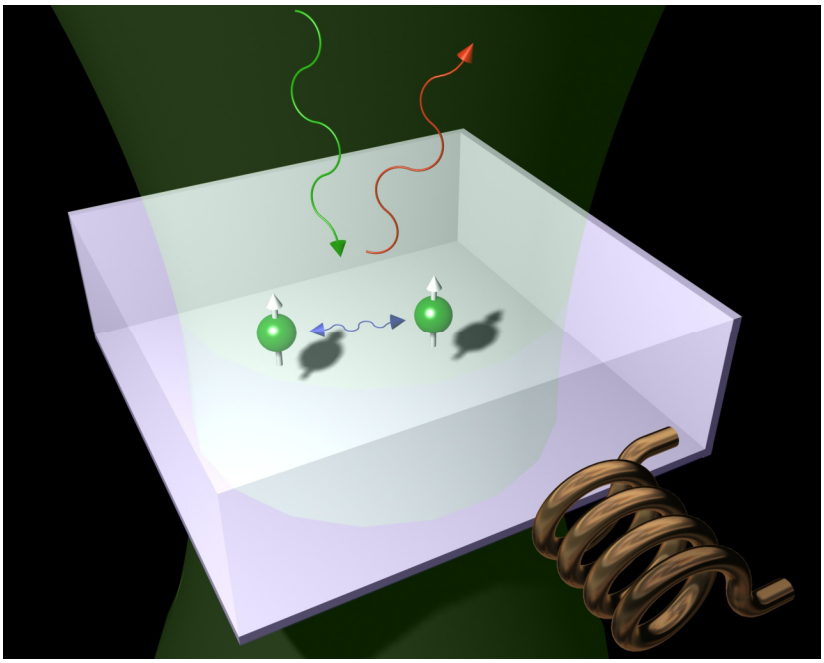


Figure 6: The interacting spins associated with single defects can be read out optically. Scattered laser photons (green, red arrows) provide information about spin states. Spin manipulation is realized using radio frequency pulses provided by microwave coil.

In summary, defects in diamond are promising systems for future quantum information technology. On short terms single photon devices based on certain colour centers have the potential to provide widely applicable devices. Quantum memories or processors certainly require advanced nanotechnologies. From the European perspective it is important to note that the world leading commercial supplier of diamond materials with unsurpassed knowledge in material production and structuring is based in Europe. In addition the perspective for room temperature device operation certainly is attractive and should be a key driving element for future research.

Conclusions

Although in its infancy, carbon based quantum processing technologies already have achieved much. The results obtained to date, and the promise of room temperature operations, set goals for other solid-state implementations. As the ITRS roadmap advances, the greater use of carbon/diamond in spintronics and other technologies will greatly aid in the push for developing carbon-based QIP.

List of terms and acronyms

Buckyball: Buckmeisterfullerene or C60, is a molecule with 60 Carbon atoms arranged in the shape of a round soccer ball.
NV: nitrogen-vacancy defect in diamond
ESR: Electron Spin Resonance, a technique to probe the local electronic environment within a molecule by irradiating a (usually) large ensemble of molecules (~10^{12}), with microwave radiation and observing the emitted re-radiation.
STM: Scanning Tunneling Microscope, a device used to image objects on atomic length scales.
ITRS: International Technology Roadmap for Semiconductors.

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Projects funded by the European Commission and related to the work in this article:

QIPDDF
A study for the construction of a Quantum Information Processing Device using Doped Fullerenes
Start date: 01/01/2000
End date: 31/12/2002
Project web site: http://www.thphys.may.ie/EC/QIPDDF/QIPDDF.htm
Contact Person: (first and last name, affiliation, email): Jason Twamley, National University of Ireland, Maynooth, Maynooth, Co. Kildare, Ireland, Jason.Twamley@nuim.ie

QIPDDF-ROSES
A study for the construction of a Quantum Information Processing Device using Doped Fullerenes and with the ReadOut of Single Electron Spin
Start date: 01/01/2003
End date: 31/12/2004
Project web site: http://www.thphys.may.ie/EC/ROSES/roeses_project.htm
Contact Person: (first and last name, affiliation, email): Jason Twamley, National University of Ireland, Maynooth, Maynooth, Co. Kildare, Ireland, Jason.Twamley@nuim.ie

Projects funded by National initiatives or organizations and related to the work in this article:

QIV
Quanteninformations-Verarbeitung
Start date: 1999
End date: 2005
Project web site http://kerr.physik.uni-erlangen.de/qiv/
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