DYNAMIC NUCLEAR POLARIZATION OF $^{15}$N@C$_{60}$ FOR QUANTUM COMPUTING

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Introduction

A scheme has recently been proposed for complete two-qubit quantum computation (QC) using pulsed ENDOR (electron-nuclear double resonance) of $^{15}$N@C$_{60}$[1]. The quantum information is stored in the electronic ($S = \frac{3}{2}$) and nuclear ($I = \frac{1}{2}$) spin states of the nitrogen atom. The first step is to prepare these spins in their ground states, which can be achieved for the electrons using a high magnetic field and a low temperature. The equilibrium nuclear polarization is always small under normal experimental conditions owing to the small nuclear magnetic moment. Dynamic nuclear polarization (DNP) can be used to transfer polarization from the electrons to the nuclei. We have performed DNP using CW ENDOR.

Experimental

$^{15}$N@C$_{60}$ was produced by the ion implantation technique described in the literature [2]. This sample was dissolved in toluene and purified with high performance liquid chromatography before being deoxygenated and sealed in an ESR tube. Continuous-wave measurements were made on a home-built CW ESR spectrometer operating at 240 GHz.

A magnetic field of 8.6 T was applied and measurements were made at 3 K. At thermal equilibrium, 98 % of the molecules have their electron spin aligned with the external field ($S_z = -\frac{3}{2}$), but 49.99 % have anti-aligned nuclear spins ($I_z = -\frac{1}{2}$). DNP consists of three steps: 1. Selectively flipping the electron spin of molecules with $I_z = -\frac{1}{2}$; 2. Flipping the nuclear spin of some of these molecules using resonant RF radiation; 3. Allowing the electron spin of these molecules to relax back to the ground state in a characteristic time $T_1$. This electronic $T_1$ time must be much shorter than the nuclear $T_1$ time in order to transfer the electron spin polarization to the nuclei.

Results and Discussion

The CW ESR of $^{15}$N@C$_{60}$ is shown in Fig. 1a. The lineshape is unavoidably saturated because $T_1 >> 1$ second. The calculated frequency of the nuclear transition for molecules with $S_z = -\frac{3}{2}$ is 47.92 kHz. This was found to be the most effective RF frequency for DNP, with the magnetic field set to coincide with the high-field resonance $I_z = -\frac{1}{2}$. Fig. 1b shows the spectrum after 20 minutes of DNP at this RF frequency. The high-field line is suppressed by ~80%, indicating that the nuclei have been successfully polarized. Larger polarizations may be achievable by exciting the other nuclear transitions.

Conclusions

DNP has been used to prepare $^{15}$N@C$_{60}$ in a state with over 80 % of the nuclei polarized. This is suitable for two-qubit QC.

Acknowledgements

This research is part of the QIP IRC (GR/S82176/01) and is supported through the Foresight LINK Award Nano-electronics at the Quantum Edge by EPSRC (GR/R660029/01) and Hitachi Europe Ltd. GADB thanks the EPSRC for a Professorial Research Fellowship (GR/S15808/01). AA is supported by the Royal Society.

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