QUANTUM MATERIALS

A chemical path to quantum information

Nanoscale graphene can be designed to function as a molecular qubit.

By **Stephen von Kugelgen and Danna E. Freedman**

The second quantum revolution is rapidly transforming fields like structural biology, cryptography, and condensed matter physics. The qubit is the core quantum unit, which has an infinite number of possible configurations through the superposition of its quantum states. This quantum property provides a unique approach for solving problems in computing, sensing, and metrology (*1*, *2*). Creating and manipulating qubits is a grand challenge, leading to a plethora of viable approaches (*3*). Spin-based molecular qubits are promising because they unify atomic scale spatial precision with structural customization for systems integration (*4*). On p. xxx of this issue, Lombardi *et al.* exemplify this approach by constructing an electronic spin-based molecular qubit from a carefully engineered state in nanoscale graphene, providing an elegant example of atomic control over qubit design (5).

The bottom-up synthesis of chemical qubits is an emerging field, with complementary metal-based and organic radical approaches delivering large advances in the past decade (*6*–*8*). Chemists can dictate the precise distribution of a qubit's spins through meticulous synthetic control over organic structures or harness ligand fields to finely tune magnetic properties at metal centers(*9*). An early example of a quantum computation was the implementation of Shor's algorithm using a nuclear spin qubit in a molecule, which highlighted the power of chemical synthesis to enforce the atomically precise relationships that control communication between elements of a quantum system (*10*). Lombardi, *et al.* showcase a previously untapped strategy in qubit engineering where their molecular qubit's unpaired spins are created not by an odd number of total electrons but rather by the precise structure of the molecule's bonding (5). They leverage the stability of aromatic π systems to promote an otherwise unfavorable bond configuration that leaves out two unpaired electrons. This enables the rational synthesis of a molecular system that replicates topological defects in graphene in a synthetically tunable platform (see the figure).

Lombardi *et al.* subject their molecule to a suite of experiments designed to both establish its viability as a qubit and elucidate the mechanisms of the collapse of the superposition state, called decoherence. The molecular system remains in a superposition state, coherence, for times that compare favorably with endohedral fullerene-based systems (*6*). The 0.33 ms coherence time that the authors observe is similar to the high values achieved with transition metal-based qubits (*8*). By subjecting the molecule to a series of microwave pulses, the authors demonstrate their control over the qubit by placing it into any arbitrary superposition of states. A benefit of chemically designing qubits is that modulating the local chemical environment can deconvolute processes that lead to the collapse of the superposition state. Lombardi *et al.* demonstrate this with experiments in solids and in solution over a wide range of temperatures, including nuclear decoupling and solvent dependence studies. This rigorous approach should serve as a guide for others vetting new chemical qubits.

A key next step toward quantum sensors is to bring chemical qubits into communication with one another or with other chemical species in a controlled fashion. Constructing multi-qubit systems with this level of precision across multiple length scales represents an outstanding challenge in the field. The first step involves progressing from isolated spin-based qubits to understanding two independently controllable, interacting qubits(*7*). To make this transition, both organic and transition metal-based approaches are promising strategies. Chemical synthesis can expand these quantum systems into many-qubit arrays. The approach from Lombardi et al. could be applied to patterned topological defects in other carbon nanomaterials. Alternatively, the bottom-up synthesized qubits could be used to forge molecular qubits into uniformly ordered arrays, by bonding them into extended framework materials, which then can be manipulated on the microscale (*11*). Extending the distances between qubits in these ordered, porous structures would not only control coherence times, but also prime them as platforms for quantum sensing of larger chemical species. Ordering qubits could be done in other interesting ways, such as using designer polymer materials like DNA to create tailored soft-matter templates (*12*).

Defect-based materials such as nitrogen vacancy pair defects in diamond are exceptional candidates for spin-based qubits. An incredible suite of spectroscopies has developed around these defects that exploit their facile optical readout(*13*). Molecular nanographene based qubits are one of many ways to create atomically precise analogues of defects than can be read out optically. Lombardi et al. show that a bottom-up approach to spin qubits is a promising strategy to expand the usefulness of this spectroscopic infrastructure. Exploiting established spectroscopic approaches by emulating the properties of defect-based systems in these synthetically tunable platforms is an exciting frontier for developing molecular qubits.

The grand challenges of quantum information science present new targets for chemical synthesis. Lombardi and coworkers model a clear path for future chemists to contribute to the advancement of the field. The authors both demonstrate a novel strategy for creating a qubit and expose its intrinsic characteristics through thoughtful application of experimental controls. Through synthetic chemistry, the insights and precision needed for new materials to transform quantum information science are within our reach.

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