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Molecular qubits: opportunities and challenges

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Highlights:

- Summarize the advantages and bottlenecks of molecular qubits.
- Demonstrate the crucial role of quantum dynamics in design of molecular qubits.
- Introduce molecular qubits as a new frontier for quantum information science.

Abstract: Quantum computing has progressed greatly, yet no current hardware platform achieves coherence preservation, precise control, and scalability at the same time. In this commentary, we consider molecular qubits as a conceptually distinct approach to quantum hardware, in which part of the required functionality can be encoded directly through chemically programmable structure rather than imposed entirely by external engineering. Owing to their atomic precision, synthetic reproducibility, tunable interactions, and diverse internal energy levels, molecular systems provide attractive opportunities for quantum information science. We review advances in molecular qubits, emphasizing their potential for uniformity, scalability, programmability, and coherence at elevated temperatures. At the same time, major challenges remain, including single-molecule readout, addressability, device integration, and the realization of high-fidelity entangling gates. We argue that the near-term impact of molecular qubits may not directly replace established platforms but instead enable hybrid architectures and promote a new paradigm of quantum hardware: the systematic chemical design of quantum function. In the long term, we may be able to address the challenges outlined in the DiVincenzo criteria and thereby enable universal quantum computation.

Keywords: molecular qubits; quantum dynamics; scalable quantum computing

1. Introduction

Quantum computing has transformed from a theoretical ambition to an increasingly competitive practical effort. Yet the central challenge of the field is no longer to demonstrate qubits. The more difficult problem is to realize qubit platforms that simultaneously achieve coherence preservation, precise control, and scalability. Despite rapid progress, no existing hardware platform has fully addressed this challenge.

Superconducting circuits, trapped ions, and solid-state defect centers have each achieved major milestones, although limitations still remain. Superconducting qubits benefit from fast gate operations and compatibility with microfabrication, but they rely on ultralow temperatures, technically challenging microwave control, increasingly complex wiring, and manufacturing-induced parameter variations as systems scale up [1–5]. Trapped ions have advantages in building relatively high-fidelity quantum gates, yet their scalability is constrained by trapping complexity, transport requirements, and interconnection challenges [6–10]. Defect-based platforms can provide localized and potentially long-lived quantum states, while reproducibility, deterministic placement, and controllable coupling are still challenging to implement [11–13]. None of these approaches are without their merits, but they all expose a common weakness of existing quantum hardware. Increasingly complex levels of engineering and control are often added.

This unresolved limitation continued to attract attention of researchers to molecular qubits. In addition to offering chemically designable two-level states with atomic precision and tunable coherence-related properties, molecular systems present a new design paradigm in which structure–property relationships are built in direct into qubit design. This makes the qubit is not only a controllable device, but also a chemically engineered object whose quantum properties can be manipulated by varying the chemical structure.

The purpose of this commentary is not to give a comprehensive review of molecular qubits. It rather examines molecular qubits as a novel hardware paradigm, in which part of the required quantum functionality can be achieved by molecular structure engineering instead of relying on external engineering entirely. We discuss the resulting opportunities, as well as the major challenges that still limit practical implementation.

2. Uniformity, scalability, programmability, and high-temperature coherence

As discussed in previous reviews of this field, such as Stefan *et al.* [14], molecular systems provide several advantages for quantum information applications. Local disorder and manufacturing-induced variation can have a significant impact on performance in many conventional platforms. In contrast, molecules are atomically precise and can be synthesized reproducibly with high uniformity, making them attractive candidates for quantum information processing. This uniformity is a foundation for scalability, as scaling up qubit number needs predictability between devices, and also makes operation easier by minimising the requirements of calibration and compensation due to manufacturing-induced variation. Another point is that molecules also offer a wealth of set of internal levels, including Zeeman splitting of electron spin, hyperfine states, and tunneling doublets. This enlarged state space allows researcher to identify and engineer computational basis which displays favorable coherence properties, such as long-lived states at comparatively higher temperatures. What is as important as previous point is that their interactions can be tuned through ligand design, coordination environment, supramolecular assembly, and symmetry control. This tunability makes molecular systems chemically programmable, thereby provides a nature path towards scalable architectures, and speed up the design of quantum gates. Molecules offer a new host for qubits with comparable uniformity, scalability, and coherence time at comparatively higher temperatures.

More importantly, molecular qubits have common design principle, irrespective of the choice of computational basis. The computational subspace (including auxiliary states) should be nearly closed,

with weak coupling to irrelevant states to avoid population leakage while ensuring addressability for quantum control. This subspace must also be shielded from external noise, especially electromagnetic fluctuations. It is essential to discover the microscopic mechanisms behind decoherence, relaxation, and crosstalk. Despite the difficulty, there are already theoretical insights into relaxation and decoherence of various molecular systems, even though they may not have been studied as qubits directly. For instance, Electron Paramagnetic Resonance (EPR) spin-relaxation studies offer insight of the factors on longitudinal relaxation time (T_1) and the dephasing mechanism for electron-spin qubits [15]. By incorporating quantum chemistry calculations, we can evaluate energy gaps between the computational basis and other levels. Wavefunction analysis yields electron density, spin density, electric dipole moments, and magnetic moments, which are key for assessing state localization, isolation, and sensitivity to external fields. Advanced vibrational analysis provides vibrational energy levels and helps suppress electron–phonon coupling, which lays the theoretical foundation for molecular engineering on scalable platforms like covalent organic framework (COF), allowing control of qubit density and inter-qubit crosstalk. Beyond static calculations, quantum dynamics simulations [16] can account for nuclear quantum effects which include state mixing due to vibrational motion [17,18], tunneling, or non-adiabatic couplings [19–23], and thus unexpected leakage can be prevented. Such simulations could also expose new quantum subspaces or coupling schemes, paving the way for novel molecular qubits. The programmability of molecular qubits, guided by these theoretical insights, enables the rational design of molecular qubits.

One of the most developed examples is molecular spin qubits. Well-defined spin centers in transition-metal coordination compounds can maintain quantum coherence at higher temperatures with high degree of tunability, which can be precisely achieved by manipulating coordination environment. A typical example is metalloporphyrins whose computational basis is defined by Zeeman splitting levels can be tuned by spin-spin interactions [24]. The main process contributing to the T_1 times is the spin-lattice relaxation process, which has been shown to strongly depend on the ligand environment, and for some systems pronounced anisotropy was observed [25]. This phenomenon indicates that the relaxation times of molecular spin qubits can be controlled by chemical synthesis and control of crystal form. Through some optimised ligand environments, relatively long coherence times have been achieved at higher temperatures, such as room temperature [26]. Scalable architectures can be created by integrating molecular qubits as building blocks into two-dimensional [27,28] or three-dimensional metal-organic frameworks (MOFs) [29]. The structure of the MOFs has been demonstrated to be able to control coherence and entanglement by tuning the phonon modes of the framework, and also the distance of the qubit spin centres, which allows tunable entanglement and chemically programmable coherence [30]. These studies are highly significant as they demonstrate that molecular qubits are not limited to theory. While single qubit readout and addressing are still a challenge, these systems can be probed and manipulated with spectroscopic techniques. These achievements give strong proof that quantum coherent behaviour can not only be induced but also be controlled in structurally controlled molecular systems, thereby paving the way towards the practical usefulness of molecular systems as hardware for quantum information science.

The electronic spins of coordinated metal centres are not the only spins that can be used to design a molecular qubit [31,32]. Stable organic radicals also provide accessible and chemically tunable spins to encode qubits. This fact is illustrated in the recent work on covalent organic frameworks. The

authors demonstrated that these organic radical qubits exhibit ultralong room-temperature spin-lattice relaxation times ($T_1 > 300$ μs at 298 K) [33]. Stable organic radicals were featured in the review of Sun *et al.* as model molecular qubit candidates [34]. They summarised that the decoherence in radical-based qubits is primarily affected by hyperfine interactions, dipolar interactions between electrons, molecular dynamics, and magnetic noise, whereas spin–lattice relaxation is dominated by spin–phonon coupling [35] via vibrational modulation of the g-tensor. These mechanisms inspire concrete design strategies like isotopic substitutions, spin-density control, dilution or spatial separation of radical centres, molecular rigidification, suppression of low-frequency vibrations, avoidance of heavy atoms, and integration into rigid COF or MOF.

Also, nuclear spins and other two-level subsystems can be used as qubit candidates. Molecular spins are an important alternative platform to electron-spin qubits [36]. Nuclear-spin qubits are also appealing as quantum memories or auxiliary qubits in hybrid electron–nuclear spin architectures, due to their long coherence times, which are provided by the relative insensitivity to magnetic noise. For instance, research on diamond Nitrogen-Vacancy (NV) centers has proven this point [37]. An even more ambitious molecular route is represented by symmetric-top molecules and related systems with intrinsically protected internal states [38]. These molecules can host qubit states derived from rotational and hyperfine structure, including K-doublet levels with extremely low dipole moment that may display reduced sensitivity to certain environmental perturbations. Particularly attractive is the possibility that their dipole moments can be effectively switched on or off depending on auxiliary states with large dipole moment, enabling state-dependent intermolecular interactions. This matters because scalable quantum information processing depends not only on protecting qubits from noise, but also on turning interactions into a controllable resource. In conventional hardware, protection and coupling are often competing design requirements. In favorable molecular systems, they may instead be co-engineered.

What's more, new types of two-level systems defining computational basis of qubit are introduced into molecular qubit design. For instance, the tunneling doublet in a double-proton tunneling system provides a well-isolated two-level system that can serve as the computational basis of a qubit [39,40]. Tunneling splitting has been observed in both the fluorobenzene-formic acid dimer and porphycene. These molecules are very analogous to the Zeeman splitting of spin states in molecular spin qubits, the resulting tunnel-split states may serve as promising qubit candidates using tunneling splitting states as computational basis. They possess appropriately spaced energy levels, allowing their manipulation to fall within the common microwave control range, from hundreds of megahertz to hundreds of gigahertz, thereby enabling a scheme for quantum gate design.

3. Challenges and future directions

Although considerable efforts have shown that molecular qubits hold great potential for exhibiting remarkable properties in quantum computing, molecular qubits are not yet a practical solution to scalable quantum computing. A molecule that performs perfectly in isolation may become technologically fragile in a device setting. Some studies have examined the key parameters in isolated molecular systems, but provides their claim of scalability often rely on idealized assumptions and still require further experimental validation. The community should also avoid overstating the chemical tunability for molecular qubits.

Closely related is the problem of integration. Molecular behavior often changes substantially when the molecule is deposited on a surface or in MOFs, which makes it difficult to find a well-characterized interface to integrate molecular qubits in a computational architecture. Additionally, one of the most immediate obstacles is readout. A molecule may be atomically precise and be arranged in a 2D/3D topology within MOF, but that does not guarantee that it can be individually initialized, addressed, and measured with fidelity, which is required for quantum information processing.

Equally important, chemically programmable coupling is not the same as a usable quantum gate. Static interaction is relatively easy to identify, while controlled high-fidelity entangling operations are much harder to realize. This gap marks the difference between a promising physical system and an operational computing platform. Some cases have shown very good properties in quantum gate design, but most of the candidates are still struggling to achieve high-fidelity entangling operations or only focus on the coherence time rather than quantum gate operation in order to compete with the other platforms. The community must also be cautious about generalizing from best-case demonstrations. Reports of unusually long coherence times or room-temperature functionality are valuable, but they do not by themselves establish broad scalability. Molecules can have remarkable properties, but these usually depend on very specific structures and environments that are hard to recreate in real, complex applications. For instance, the relaxation time (T_1) is measured through electron paramagnetic resonance in the cases of molecular spin qubits, which means that the sample preparation and instrument status can strongly influence the properties we want to measure, as single qubit measurement is still impossible. What's more, the T_1 observed in ensemble measurements like EPR may not reliably reflect the T_1 of isolated molecular qubits, because the interaction in samples may influence the relaxation process of qubits. For systems reported to introduce new types of two-level systems defining computational basis of qubit, community should remain cautious, as this interpretation may come from theoretical deduction rather than experimental validation.

For these reasons, molecular qubits may not directly replace superconducting circuits or trapped ions as universal quantum computing platforms in the short term. A more realistic and potentially more valuable perspective is that they will first serve as specialized components in hybrid quantum technologies—such as quantum memories, tunable couplers, or chemically programmable systems for sensing and simulation. In a more general sense, they might also find their most impactful contribution in a methodological one: molecular qubits encourage the community to move away from the discovery of useful quantum materials and to the design of quantum functions. In the long run, molecular qubits can also be a path to universal quantum computation, if one can overcome the following challenges.

If analysed in the light of the DiVincenzo criteria [41], the priorities for future research are therefore clear. Single-molecule readout and addressability have to become major goals, since these are the key challenges to fully realise the success of atomic precision and scalability. Stable and well-characterized molecule–device interfaces are essential if chemical precision is to be retained during technological integration. However, the next step for the community is to progress from coherence benchmarks to concrete demonstrations of universal quantum gate sets and qubit initialisation procedures. Most importantly, molecular design should be more architecture-driven than novelty-driven, with fault tolerance, control protocols and scalable architectures in mind.

Molecular qubits are not a complete solution to scalable quantum computing. One of the most

unambiguous indicators, however, that the field might need something more than improved fabrication to solve its hardware constraints is their existence. Molecular systems offer a unique path to scalable quantum computation, one that starts not with complex devices, but with improved building blocks through the use of chemically designed coherence, protection and coupling.

Declaration of generative AI and AI-assisted technologies

During the preparation of this manuscript, the authors used AI-assisted technologies only to improve language and readability. Specifically, the authors used Grammarly for language polishing only in limited sections. The authors take full responsibility for the content of the manuscript.

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Authors' contribution

Conceptualization, X.Z. and W.B.; investigation, X.Z. and W.B.; resources, W.B.; writing—original draft preparation, X.Z. and W.B.; writing—review and editing, X.Z. and W.B.; supervision, W.B.; project administration, W.B.; funding acquisition, W.B. All authors have read and agreed to the published version of the manuscript. All authors have read and agreed to the published version of the manuscript.

Conflicts of interest

Wensheng Bian holds the position of Associate Editor for *Quantum Research* and has not been peer-reviewed or made any editorial decisions for this paper. The authors declare no conflicts of interest.

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