Molecular Qubits Based on Zwitterions with Close pKa Values and Comparable Charge-Transfer Energies: A Theoretical Analysis

Dr. Omar González-Santiago

Affiliation: Graduate in Pharmacy Coordination, Faculty of Chemical Science, Universidad Autónoma de Nuevo León.

Adress: Av. Universidad s/n, Ciudad Universitaria, San Nicolas de los Garza, Nuevo León, México.
Correspondence: omar.gonzalezst@uanl.edu.mx
ORCID: https://orcid.org/0000-0003-1841-1783

Abstract

This theoretical analysis proposes zwitterionic compounds as molecular qubits. Organic zwitterions are characterized by functional groups with closely spaced pKa values, while inorganic or hybrid zwitterions exhibit comparable charge transfer energies between two internal centers. In organic systems, the strategic proximity of pKa values enables precise control over protonation states, facilitating the representation of quantum basis states |0⟩ and |1⟩, as well as superposition states within individual molecules. In inorganic systems, discrete quantum states arise from charge localization at distinct centers, with superposition resulting from partial charge delocalization. The essential characteristics of an ideal zwitterionic molecule for encoding quantum information are discussed. While the primary application lies in quantum computing, other potential uses are not excluded.

Keywords: Zwitterions, Qubits, Molecular qubits, Quantum computing.

Introduction

Implementations of quantum computing have primarily focused on physical systems such as superconducting circuits, trapped ions, or photons to create qubits. While these platforms have shown significant advances, they continue to present challenges related to scalability, miniaturization, and integration into complex systems [1]. This has motivated the search for alternative qubit platforms, including molecular and chemical systems, which offer a path toward high-density information storage at the nanometric scale [2]. Previous studies on spin-based molecular qubits and quantum simulation using chemical systems reinforce the viability of quantum information processing at the molecular scale [3,4].

The objective of this theoretical study is to present a theoretical framework for molecular qubits based on zwitterions. The desired characteristics of an ideal zwitterionic system for molecular quantum computing are discussed, laying the foundations for its theoretical and experimental validation.

Development

Zwitterions are molecules that exhibit spatially separated positive and negative charges. Their protonation equilibria can be influenced by environmental parameters such as pH, temperature, and ionic strength, suggesting a mechanism for accessing discrete, quantum-analogous states within a single molecular entity [5,6]. Common amino acids serve as illustrative examples of zwitterions, noting that their pKa values are typically widely separated: Glycine (NH_2CH_2COOH) – pKa (carboxyl): 2.34, pKa (amino): 9.60 Alanine ($CH_3CH(NH_2)COOH$) – pKa (carboxyl): 2.34, pKa (amino): 9.69 Serine ($HOCH_2CH(NH_2)COOH$) – pKa (carboxyl): 2.21, pKa (amino): 9.15 Cysteine ($HSCH_2CH(NH_2)COOH$) – pKa (carboxyl): 1.71, pKa (amino): 10.78 [7].

Conceptual Framework and Proposed Mechanism

A zwitterion possessing two functional centers (one acidic/basic in organic systems or one cationic/anionic in inorganic systems) with close energetic parameters could encode quantum information according to the following scheme: State $|0\rangle$: in organic zwitterions, the acidic group is protonated and the basic group deprotonated; in inorganic zwitterions, the positive charge is localized at center A, while the negative resides at center B. State |1⟩: in organic zwitterions, the acidic group is deprotonated and the basic group protonated; in inorganic zwitterions, the charge distribution is inverted between centers A and B. Superposition (|S⟩): intermediate state where the molecule exhibits characteristics of both |0⟩ and |1⟩; in organic zwitterions, this corresponds to partial protonation, while in inorganic zwitterions it corresponds to partial charge delocalization between both centers [6].

In both organic and inorganic systems, quantum superposition is conceptually represented as a dynamic equilibrium between two energetically comparable states. For organic zwitterions, environmental factors such as pH, temperature, and ionic strength govern the protonation equilibrium, with protonic tautomerism as a state transition mechanism [7]. For inorganic zwitterions or hybrid organometallic systems, analogous control can be achieved through external stimuli such as electric fields, ligand coordination, or thermal modulation, which influence the internal charge distribution.

All of the above suggests a pathway for chemical or physical manipulation of molecular qubits. Maintaining coherence will critically depend on achieving exceptional environmental stability to mitigate sources of decoherence, including molecular vibrations, solvent interactions, and thermal fluctuations. Related concepts such as proton-coupled electron transfer and charge transfer equilibria in molecules provide useful analogies for designing switchable quantum states [8,9].

Ideal Properties of Zwitterions for Acting as Qubits

For zwitterions to function effectively as molecular qubits, they should ideally meet the following criteria:

- Close pKa values in organic systems or comparable charge transfer energies in inorganic systems.
- Chemical stability, resisting degradation, oxidation, or unwanted reactions.
- Molecular rigidity that minimizes decoherence induced by internal vibrations.

- Environmental compatibility, including sufficient solubility and stability in the relevant experimental medium [11,12].

Extensions to Inorganic Zwitterions

Some inorganic or hybrid organometallic species exhibit internal charge separation that can support qubit encoding. Examples include:

- Phosphonium–borate systems ($R_3P^+–BR_3^−$) [13].
- Carborane clusters with charged substituents [14].
- Polyphosphazene chains with alternating cationic and anionic centers [15].

These systems may not have classical pKa values in aqueous solution but exhibit effective protonation or charge transfer equilibria analogous to organic zwitterions. They offer advantages such as rigid geometries, greater thermal and chemical stability, and intrinsic internal electric fields that can reduce decoherence.

Advantages and Potential Applications

Molecular qubits based on zwitterions offer several advantages. Single-molecule qubits enable exceptionally high information density at the nanometric scale [2]. Their protonation states (organic) or charge distributions (inorganic) are modulable through chemical or physical stimuli, enabling versatile state initialization and control [12]. The intrinsic chemical or electronic equilibrium provides a direct analog to quantum superposition, representing quantum states within a tangible molecular framework [17].

Hybrid molecular qubits could integrate chemical precision with device-based scalability, and structural tuning of molecules would allow designing customized Hamiltonians for specific quantum computing applications [2].

Challenges and Future Studies

Decoherence arising from solvent interactions, molecular vibrations, and environmental noise constitutes a major challenge [1], as does controlling the local environment (pH, temperature, ionic strength, or electric fields). The development of reversible and non-destructive manipulation techniques for protonation or charge localization is also essential.

Future work should prioritize theoretical simulations and quantum-chemical modeling to evaluate the proposed zwitterions, examining how chemical or electronic properties influence superposition lifetimes and coherence. The synthesis of optimized zwitterions with close pKa values or comparable charge transfer energies will enable experimental validation. Success could lead to their incorporation into hybrid quantum architectures, and quantum sensing techniques could improve state readout [19].

Conclusions

Zwitterionic molecules provide a theoretically promising platform for molecular qubits. Organic zwitterions illustrate the principle through protonation equilibria, while inorganic or hybrid zwitterions extend the concept through comparable charge transfer energies between centers. Both systems allow the representation of quantum superposition states. This theoretical analysis warrants further theoretical and experimental exploration to confirm whether zwitterions could be applied as molecular qubits.

Conflict of interests: The author declares no conflict of interest.

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