Quantum Logic Gates Based on DNAtronics, RNAtronics, and Proteintronics

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Quantum computers (QCs) adopt an n-state quantum mechanical system to manipulate the superposition state. However, molecular transistors are not used to build up the quantum logic gate. Herein, it is demonstrated that DNA, RNA, and protein are promising media for QCs, and one uses residue pairs, including nucleotide base pairs and amino acid pairs, via proton-coupled electron transfer to fabricate a quantum logic gate. In the residue pair, the proton transfer between donor and acceptor states fulfills a qubit. Both the DNA-CG (3-qubit) nucleobase pair and nucleotide base pair obey the Toffoli gate. AT (2-qubit) nucleotide base pair behaves as a SWAP gate and a CNOT gate. Furthermore, the AU and RNA-CG nucleotide base pairs follow the CNOT gate and Toffoli gate, respectively. In addition, a pair of amino acids achieves 1-qubit and satisfies the Pauli-X, -Y, and -Z gates. The generators of universal quantum logic gates are obtained.

1. Introduction

A quantum computer (QC) [1–3] implements quantum bits (qubits) and qudits [4] (e.g., qutrits [5] and ququarts [6]) to conduct computations instead of a traditional digital computer built from a transistor in which a binary bit is represented by either 1 or 0. Based on the Church–Turing–Deutsch principle, a computing machine conducts simulations of every physical process and behaves as a universal QC. [7–9] Unlike a classical bit, the basic unit of a qubit is the superposition $\psi = c_0 |0 \rangle + c_1 |1 \rangle$ of two qubit states, |0⟩ and |1⟩, where $c_0$ and $c_1$ denote complex numbers. [10] However, the operation of a QC with a relatively large number of qubits for conducting universal computations has attracted considerable attention. [11]

Using quantum algorithms such as Shor’s algorithm [12] or a quantum many-body simulation [10] and Simon’s algorithm [13] a large-scale QC could tackle problems faster than a classical computer. Until now, present quantum algorithms have been implemented by superconducting flux qubits (D-wave systems) [14], nuclear magnetic resonance (NMR) techniques [15,16], and photonic QCs [17] as well as ion-trap systems [18,19] For NMR techniques, Shor’s factorizing algorithm, [20] which uses seven qubits, has been applied. The qubits are encoded in mixed states, and the output is a result of an ensemble measurement. Hence, NMR QCs are not scalable. [21] For a trapped-ion QC, the qubits are stored in the electronic states of ions and are controllable in long-lived internal states, and their quantum states can be detected with a very high efficiency close to 100%. [19,22,23] These characteristics permit the manipulation of pure states to build a scalable and universal QC. [24] Nevertheless, no quantum logic gate has been executed with a subnano-scaled molecular transistor to date.

Classical computers operate with a microprocessor that consists of semiconductor logic gates with electronic input and output signals of a binary digital nature. The output can be only one of the two states, on or off, corresponding to logic 1 or 0, respectively. Consequently, the signal pattern can be described by a truth table based on Boolean algebra. [25] This critical feature in constructing computers could be conducted by a single-molecule transistor as a future classical computer. [26,27] However, accomplishing concerted arrays of molecular transistors remains an intrinsic challenge. [28,29]

Recently, several experiments have shown the feasibility of conducting computations at the molecular level. For example, DNA is a reliable biomolecule and can be used to build molecular computation systems; however, it was used as a classical liquid computer to solve the Hamiltonian path problem. [30] DNA-based logic gates [25,31] have been designed by deoxyribozyme ligases. [32,33] It is possible to integrate the logic gates into simple circuits using a series of deoxyribozyme ligases communicating via a deoxyribozyme phosphodiesterase. [38] Meanwhile, NOT and two-input AND gates were integrated into an INHIBIT logic gate, and signal transduction was mediated by the association of several DNA strands. [34] The classical liquid computer...
manipulates a very large molecule in solution, and the speed of computation is slow.\textsuperscript{[33]}

It is feasible that with the significant miniaturization of individual molecular logic elements,\textsuperscript{[27,36]} these small devices can reduce energy and material consumption.\textsuperscript{[37]} Nucleic acids have been considered to be promising molecules for constructing molecular devices including logic gates due to the highly selective and predictable interactions among the Watson–Crick base pairs, namely, AT, CG, AU, and GU, (A: adenine, C: cytosine, G: guanine, T: thymine, and U: uracil).\textsuperscript{[25]} Thus, to use biomolecules as quantum logic gates, the proposition of a bottom-up approach toward the design of electronics at the molecular level is attractive.

The designation of available molecular logic gates becomes highly attractive in molecular computing. In this article, we report that the residue pairs, including nucleic acids and amino acids, are potential candidates as a quantum logic gate in a transistor rather than as a classical liquid computer. The proton-coupled electron transfer (PCET) theory provides a different approach for a two-state system instead of NMR and trapped-ion methods. This method is analogous to a conventional microprocessor using an elementary logic gate to operate electronic circuits that obey Boolean logics.\textsuperscript{[38]}

To go beyond a nucleic acid-based classical liquid computer, DNA electronics (DNAtronics) was considered, and our results show that the nucleotide base pairs obey the Toffoli, CNOT, and SWAP gates in the QC.\textsuperscript{[39]} Moreover, in RNA electronics (RNAtronics), Toffoli and CNOT gates are found. Thus, it is possible to implement these quantum logic gates in the microprocessor through a molecular junction or transistor device. To fulfill the universal QC requirement, the 1-qubit controlled by proton transfer can be found in an amino acid pair that satisfies Pauli-X, -Y, and -Z gates.

In general, the pK\textsubscript{a} of phosphate groups in the phosphodiester backbone is close to zero, and they are negatively charged with a −1 charge state at pH 7. For an individual nucleotide base pair, the protonated/deprotonated state of the phosphate group can be controlled by the pH value, which dominates its charge state. Our study shows that there is an obvious transmission spectrum (TS) change for each individual nucleotide base pair at different charged phosphate groups, which confirms that the type of quantum logic gate of the nucleotide base pairs is pH dependent.

2. Results and Discussion

2.1. Proton Transfer Potential Energy Surface

We studied the proton transfer potential energy surface of nucleotide base pairs, including DNA base pairs (AT and CG) and RNA base pairs (CG, AU, and GU), in vacuum and solution. All molecular junctions of the nucleotide base pairs are shown in Figure 1. The experimental feasibility of the methodology has been described in our previous studies.\textsuperscript{[40]} Let us consider an hydrogen (H) bond in the nucleotide base pair and define the proton transfer from a native state (the donor state, i.e., N—H⋯O(N)) to its conjugated state (the acceptor state, i.e., N⋯H—O(N)). For example, there are two H bonds in the AN\textsubscript{N}—H\textsubscript{1}⋯O\textsubscript{N} and A\textsubscript{N}N—H\textsubscript{2}⋯O\textsubscript{N} base pair, where both proton H\textsubscript{1} and proton H\textsubscript{2} simultaneously at the donor (acceptor) state are denoted as DD\textsubscript{XT} (AA\textsubscript{XT}) and so on (see definition in Table S1, Supporting Information). Here, the donor (acceptor) state can be defined as either |0⟩ (|1⟩) or |1⟩ (|0⟩).

According to the transition rate theory,\textsuperscript{[41]} if the energy barrier of a double-well potential energy surface is large enough, i.e., barrier height/k\textsubscript{B}T > 3.5,\textsuperscript{[42]} (k\textsubscript{B}: the Boltzmann constant and T: the absolute temperature), then, it exhibits a transition rate and two distinct states, |0⟩ and |1⟩. Otherwise, if the energy barrier is small or close to thermal energy k\textsubscript{B}T, then the two states are indistinguishable and proceed on coherent motion. Alternatively, the first passage time analysis might be applied to measure the transition time instead of the transition rate. In vacuum, our calculated results indicate that there is an asymmetric double-well potential energy surface for proton transfer from the donor state to the acceptor state, and the barrier

![Figure 1](image-url). Molecular junctions of the nucleotide base pairs. a) DNA: A=T, b) DNA: C=G, c) RNA: C=G, d) RNA: A=U, and e) RNA: G=U. The nucleotide base pairs (O: red, N: blue, C: cyan, P: dark gray, and H: light gray) were wired to the Au electrodes (golden) through the S atom (yellow). The source, scatter, and drain components are the left electrode, the nucleotide base pairs, and the right electrode, respectively.
height $\Delta G_D$ is much higher than 18.0 kcal mol$^{-1}$; in contrast, the barrier height $\Delta G_A$ is less than 6.0 kcal mol$^{-1}$ (Figure S1 and Table S2, Supporting Information). The process of proton transfer in the nucleotide base pair satisfies barrier height $k_BT > 3.5$ and agrees with the two local minimum states (Figure S1a1–a5, Supporting Information). In Appendix A, a detailed theoretical analysis of an asymmetric double-well system applied to the proton transfer along the H bond in vacuum was developed to prove the existence of the superposition of two qubit states $|0\rangle$ and $|1\rangle$ (Figure S2, Supporting Information).

When the density functional theory (DFT) computation was executed for the nucleotide base pair in solution, the solvent degrees of freedom were averaged to obtain an effective potential.[43,44] Notably, the effective barrier height is larger in solution than in vacuum (Figure S1, Supporting Information). We confirm that the two distinct states are signified during proton transfer in the nucleotide base pairs. To consider the process of proton transfer in solution, the analytic transition rate theory[45] based on the spin-boson model is used to include the solvent degrees of freedom; thus, a superposition state of $c_0|0\rangle + c_1|1\rangle$ is obtained, where $c_0$ and $c_1$ are complex amplitudes, depending on the temperature and barrier height (Appendix B and Figure S2, Supporting Information). At room temperature, the thermal energy $k_BT$ is approximately $0.593$ kcal mol$^{-1}$, and the $\Delta G_D/k_BT$ value is large enough to permit the existence of two states $|0\rangle$ and $|1\rangle$. Substantially, we validate that qubit states exist in solution at low or finite temperatures.

Because protons are heavier than electrons, protons have a longer tunneling time $\tau$, i.e., $\tau \propto (\text{particle mass})^{-1/2}$.[45,46] The PCET timescale relies on proton tunneling and is approximately $43$ times longer than the pure electron transfer (ET) time scale. Based on the PCET process,[47] DNAtronics and RNAtronics are a pure and scalable state in vacuum, but they are a mixed and nonscalable state in solution at finite temperature.[48] Therefore, the nucleic acids display an assembly of qubit arrays not only in vacuum but also in solution.

2.2. Logic Gates of the Nucleotide Base Pairs

To better understand the behavior of ET, it is necessary to calculate the TS of the nucleotide base pairs (i.e., AT, CG, AU, and GU). The threshold for ET is $TS(D_j) > 0.05$, and each configuration was at the optimized distance $d_{\text{N-O}}$, where $d_{\text{N-O}}$ is the distance between the H bond donor and acceptor, for example, $d_{\text{N-O}}$ in $\text{N}4\text{H}\cdots\text{O}2\text{p}$. We found that the TS patterns were almost identical for the mirror images, i.e., $\text{DD}_{\text{AT}}$ and $\text{DD}_{\text{TA}}$ (Figure S3a1–d1 and a2–d2, Supporting Information). This result illustrates that the ET process of the nucleotide pair is direction independent and is a symmetric ET process; in contrast, the polypeptide chain ET process is direction dependent.[49] Consistently, the potential energy surface of proton transfer is a double-well surface, and the electronic state can be a superposition of two qubit states, $|0\rangle$ and $|1\rangle$. For two H bond AT nucleobase pairs, $\text{DA}_{\text{AT}}, \text{DD}_{\text{AT}}, \text{AA}_{\text{AT}},$ and $\text{AD}_{\text{AT}}$ are denoted as $|00\rangle$, $|01\rangle$, $|10\rangle$, and $|11\rangle$ states, respectively, meaning that AT is a 2-qubit state. The TS/density of states (DOS) were calculated for each state, and the corresponding truth table is shown (Figure S3a3–d3, Supporting Information and Table 1). In the $\text{DA}_{\text{AT}}$ state, the two protons are close to the source electrode, and $TS(D_j)$ is zero, whereas the truth table represents the input $|xy\rangle = |00\rangle$ and output $|z\rangle = |0\rangle$. When proton $H_2$ is transferred from the $\text{DA}_{\text{AT}}$ state to the $\text{DD}_{\text{AT}}$ state where ET occurs, there are apparent peaks on $TS(D_j)$ and the DOS within the $D_j$ region (Figure S4a,b, Supporting Information), and the truth table shows input $|xy\rangle = |01\rangle$ and output $|z\rangle = |1\rangle$. The molecular orbital (MO) displays an obvious migration of the electron density distribution from the highest occupied molecular orbital (HOMO) to the extended lowest unoccupied molecular orbital (LUMO) across the molecular junction and the interface S atom of the drain electrode (Figure S4c, Supporting Information). Notably, charge separation is controlled by proton transfer in the H bond. A further analysis of the $N_e\cdotsH_1\cdotsO_4$ and $N_1\cdotsH_2\cdotsN_5$ atomic orbitals (AOs) for the $\text{DD}_{\text{AT}}$ state shows that there is a high electron density overlap for $N_6\cdotsO_4$ and $N_7\cdotsN_8$, whereas protons $H_1$ and $H_2$ are transferred. In particular, electrons mainly pass through the $2p_y$ orbital overlap between the H-bonding donor and acceptor, N atom or (N) O atom (Figure S4d, Supporting Information). We confirm that no electron density was observed in the $H_1$ and $H_2$ AOs; hence, $H_1$ and $H_2$ are in the proton state rather than in the hydrogen state. Our results show that AT and AU nucleobase pairs are classical logic gates, including OR, NOR, AND, or NAND, and the CG nucleobase pair obeys the quantum Toffoli logic gate, i.e., 3-qubit gates, but the GU nucleobase pair does not.

2.3. Logic Gates of the Nucleotide Base Pairs

The nucleic acids are composed of nucleotides, which are made up of a nucleobase, five-carbon sugar ribose or deoxyribose, and a phosphate group. To create a logic gate based on the ET of nucleic acids, we consider a nucleotide base pair as a basic building block of a processor (Figure 1). Notably, the charges of the phosphate groups on an individual nucleotide base pair depend on the pH value of the environment. For a nucleotide base pair, the two phosphate groups $L\cdots\text{PO}_4^2−/R\cdots\text{PO}_4^2−$ are negatively charged ($−1, −1$) under physiological conditions or at neutral solution pH 7, where L (R) denotes the source (drain) electrode. Interestingly, we study whether nucleotide base pairs exhibit quantum logic gate behavior.

2.3.1. AT Nucleotide Base Pair

First, the spin effects on TS of the AT nucleotide base pair with the phosphate group charge ($−1, −1$) in the singlet state, triplet state, and quintet state were studied (Figure S5, Supporting Information). In the singlet state, when the proton $H_1$ is transferred from the $\text{DA}_{\text{AT}}$ state to the $\text{AA}_{\text{AT}}$ state, the intensity of $TS(D_j)$ changes from zero to nonzero, corresponding to an output $|z\rangle = |1\rangle$ of the logic gate. The $\text{DA}_{\text{AT}}$ and $\text{AD}_{\text{AT}}$ states also have explicit $TS(D_j)$ intensities and output $|z\rangle = |1\rangle$. Under this circumstance, the truth table shows that the AT nucleotide base pair obeys a classical logic gate (Table 2). However, in the triplet state, classical gates, such as XNOR or XOR, or a quantum CNOT gate, and in the quintet state, classical logic gates are obeyed (Figure S5, Supporting Information and Table 2).
Table 1. Truth table of the nucleobase pairs.

| Nucleobase pair | AT | CG | AU | GU |
|-----------------|----|----|----|----|
|                  | State | In | Out | State | In | Out | State | In | Out | State | In | Out |
|                  | x | y | z | x | y | z | x | y | z | x | y | z | x | y | z | x | y | z | x | y | z |
| DA_AT            | 0 0 0 | DDA_CG | 0 0 0 | DDA_AU | 0 0 0 | DDA_GU | 0 0 0 |
| DD_AT            | 0 1 1 | DDD_CG | 0 1 0 | DDD_AU | 0 1 0 | DDD_GU | 0 1 0 |
| AA_AT            | 1 0 1 | DAA_CG | 0 1 0 | DAA_AU | 1 0 0 | DAA_GU | 1 0 0 |
| AD_AT            | 1 1 1 | DAD_CG | 1 1 1 | DAD_AU | 1 1 1 | DAD_GU | 1 1 0 |

Logic gate

| classical OR or NOR or AND or NAND | Toffoli | classical OR or NOR or AND or NAND | none |
|-----------------------------------|--------|-----------------------------------|------|

Table 2. Spin effect on the truth table of the AT nucleotide base pair with the phosphate group charge (−1, −1).

| AT nucleotide base pair with the phosphate group charges (−1, −1) |
|---------------------------------------------------------------|
| Spin state                                                   |
| Singlet                                                      |
| state                  | In | Out | state | In | Out | state | In | Out | state | In | Out |
|-----------------------|----|-----|-------|----|-----|-------|----|-----|-------|----|-----|
| DA_AT                 | 0 0 0 | DDA_CG | 0 0 0 | DDA_AU | 0 0 0 | DDA_GU | 0 0 0 |
| DD_AT                 | 0 1 1 | DDD_CG | 0 1 0 | DDD_AU | 0 1 0 | DDD_GU | 0 1 0 |
| AA_AT                 | 1 0 1 | DAA_CG | 0 1 0 | DAA_AU | 1 0 0 | DAA_GU | 1 0 0 |
| AD_AT                 | 1 1 1 | DAD_CG | 1 1 1 | DAD_AU | 1 1 1 | DAD_GU | 1 1 0 |

Table 2. Spin effect on the truth table of the AT nucleotide base pair with the phosphate group charge (−1, −1).

The distance \(d(N_6…O_4) = 2.934 \text{ Å}\). For the high spin states, \(\alpha\) and \(\beta\) indicate the spin-up and spin-down states, corresponding to the spin-polarized current \(I_{\parallel}\) and \(I_{\perp}\), respectively. If \(T_{\parallel}(D_0) \neq 0\), then \(l_{\parallel} \neq 0\); otherwise, it is zero. The charge current \(I_{\perp} = I_{\parallel} + I_{\perp}\) determines the output state, when \(I_{\perp} \neq 0\), the output state is \(|1\rangle\). \(|z\rangle\) is the output state measured by \(l_{\perp} = l_{\parallel} + l_{\perp}\).
Therefore, the spin effect of the AT nucleotide base pairs shows that quantum CNOT and classical logic gates are observed.

As the charge of the phosphate group depends on the pH value in the environment, we can examine the behavior of the quantum logic gate of the nucleotide base pairs by changing the pH value or the protonation of the phosphate group. Subsequently, the charge effect of the phosphate group on the TS/DOS of the AT nucleotide base pair in the singlet state was studied to obtain the truth table (Figure S6, Supporting Information and Table 3). The truth table shows that the AT nucleotide base pairs with phosphate charges (0, 0), (−1, −1), (0, −1), and (−2, 0) are classical logic gates; charges (−1, 0), (0, −2), and (−2, −2) are quantum SWAP gates; and charges (−1, −2) and (−2, −1) are none. The charge (−1, −1) is the classical logic gate, whereas the charge of the phosphate group on the AT nucleotide base pair can be controlled to generate a quantum logic gate. In other words, the quantum logic gate of the nucleotide base pair depends on the pH effect.

Next, the natural bond orbital (NBO) charge distribution was analyzed by Gaussian program to calculate the natural charge (NC) of each site in the nucleotide base pair for all the charge states (Figure S7a–i, Supporting Information). If one (or two) proton is transferred, i.e., DAₜᵣₜ → DDₜᵣₜ (or ADₜᵣₜ), then the transferred electron charge is defined as

\[ e_{ET} = L_{initial} - L_{final} + 1.0 \text{ (or 2.0)} \]

so that the charge in the nucleotide attached to the source electrode is equal to the charge in the nucleotide attached to the drain electrode, where \( L_{initial} \) and \( L_{final} \) denote the NC of the nucleotide attached to the source and drain electrodes at the initial (final) ET state, respectively. For example, with the phosphate group charge (−1, −1) in the singlet state, the NC of the DDₜᵣₜ state is mainly distributed in the adenine group (M1) (Figure S7i, Supporting Information). While a proton is transferred from the DDₜᵣₜ state to the ADₜᵣₜ state, the NC (or electron) migrates from thymine (M2) to adenine (M1). Explicitly, this confirms the PCET process that once a proton with one unit of positive charge is transferred forward, an electron moves backward.

### 2.3.2. DNA-CG Nucleotide Base Pair

In the DNA-CG nucleotide base pair, there are three H bonds, termed 3-qubits, and there are 2³ possible combinations of D and A states in the proton transfer states. All TS/DOS and truth tables of the DNA-CG nucleotide base pair associated with the spin states and the phosphate group charges are presented (Figure S8, S9 and Tables S3-S4, Supporting Information). With the phosphate group charge (−1, −1) in the singlet state, only four states have TS(Dₜᵣₜ) ≠ 0, proving that the DNA-CG

| State | In | Out |
|-------|----|-----|
|       | x  | y   | z'  | z'  | x'  | y'  |
| DAₜᵣₜ | 0  | 0   | 0   | 0   | 0   | 0   |
| DDₜᵣₜ | 0  | 1   | 1   | 0   | 1   | 0   |
| AAₜᵣₜ | 1  | 0   | 1   | 0   | 0   | 1   |
| ADₜᵣₜ | 1  | 1   | 1   | 1   | 1   | 1   |

| Logic gate | Classical OR or NOR or AND or NAND | Classical OR or NOR or AND or NAND | SWAP | Classical OR or NOR or AND or NAND | SWAP |
|------------|------------------------------------|------------------------------------|------|------------------------------------|------|
| DAₜᵣₜ      | None                               | None                               | SWAP | None                               | None |

| State | In | Out |
|-------|----|-----|
|       | x  | y   | z'  | z'  | z'  | y'  |
| DAₜᵣₜ | 0  | 0   | 1   | 1   | 0   | 0   |
| DDₜᵣₜ | 0  | 1   | 0   | 1   | 0   | 0   |
| AAₜᵣₜ | 1  | 0   | 0   | 1   | 0   | 1   |
| ADₜᵣₜ | 1  | 1   | 0   | 1   | 0   | 1   |

| Logic gate | Classical OR or NOR or AND or NAND |
|------------|------------------------------------|
| None       | None                               |

*Distance \(d(N₆…O₄) = 2.934 \text{ Å} \).
nucleotide base pair obeys the quantum Toffoli gate. In contrast, with the higher spin states and the other charged phosphate groups, the DNA-CG nucleotide base pair does not follow a quantum logic gate. Compared with the $TS(D_j)$ intensity of the CG nucleobase pair, the $TS(D_j)$ intensity of the DNA-CG nucleotide base pair is weaker. This result is attributed to the charge distribution by the presence of the phosphate and ribose (deoxyribose) groups. Thus, the phosphate and ribose (deoxyribose) groups play a crucial role in attenuating ET. Nevertheless, both the DNA-CG nucleobase pair and nucleotide base pair in neutral solution have the potential to be a quantum logic gate. Similarly, the NBO charge distribution of each site in the nucleotide base pair for all the charged states was calculated (Figure S10a–i, Supporting Information). For example, when a proton is transferred from the DDD$_{CG}$ state to the ADD$_{CG}$ state with phosphate group charges ($-1, -1$), the $TS(D_j)$ intensity changes to zero, and the NC of the cytosine base (M1) is increased (Figure S10i, Supporting Information). The proton transfer process, DAA$_{CG} \rightarrow$ DDA$_{CG} \rightarrow$ ADA$_{CG}$, manifests that the NC is transferred from cytosine (M1) to guanine (M2) and TS(DE) $\neq 0$. In this system, the NBO analysis illustrates the mechanism of PCET.

For a Toffoli 3-qubit gate, the input and output are given as $|xyz\rangle$ and $|x'y'z'\rangle$ states, respectively. Here, $|x'\rangle = |xy\rangle$ is obeyed, where $x$ and $y$ are in the orthogonal directions and can be probed by NMR methods experimentally (Figure 2).[49-53] Recently, the advanced single-molecule NMR technique at atomic resolution has reported that a few or even individual nuclear spins can be probed, where a single nuclear spin procession can be tracked using periodic weak measurements.[52,53] Accordingly, the $|x'\rangle$ and $|y'\rangle$ states for the output $|x'y'z'\rangle$ state can be determined. Similarly, for a SWAP 2-qubit gate, the input and output are $|xy\rangle$ and $|x'y'\rangle$ states, respectively, by definition $|x'\rangle = |xy\rangle$. However, the $|x'\rangle$ state can be probed from the input $y$-state by the single-molecule NMR method, and the $|y'\rangle$ state can be obtained from the $x$-state by our molecular junction method.

### 2.3.3. RNA Nucleotide Base Pairs

The sugar in DNA and RNA is different, i.e., DNA is deoxyribose and RNA is oxyribose. The TS/DOS of three RNA nucleotide base pairs (AU, CG, and GU) in the singlet state with the phosphate charge group $(-1, -1)$ were calculated, and the truth table

![Figure 2. Illustration of the experimental measurement for the proton position and the logic gate states. a) A molecular junction of CG 3-qubit logic gate. The proton position can be probed by the nitrogen-defected (NV) diamond dot as a spin sensor and a microscope. The nucleotide base pairs were wired to the Au electrodes (source and drain). b) The device image of a Toffoli gate based on CG 3-qubit. The input and output logic levels are illustrated where a single nuclear spin procession can be tracked by NMR methods experimentally. c) A 3-qubit circuit diagram.](image-url)

### Table 4. Truth table of the RNA nucleotide base pairs with the phosphate group charge $(-1, -1)$ in the singlet state.

| RNA nucleotide base pair with the phosphate group charges $(-1, -1)$ | State | In | Out | State | In | Out | State | In | Out |
|---|---|---|---|---|---|---|---|---|---|
| | | $x$ | $y$ | $y'$ | | $x$ | $y$ | $y'$ | | $x$ | $y$ | $z$ | $z'$ |
| AU | DDA$_{AU}$ | 0 | 0 | 1 | DDA$_{GU}$ | 0 | 0 | 0 | DDA$_{CG}$ | 0 | 0 | 0 | 0 |
| | DA$_{AU}$ | 0 | 1 | 0 | DA$_{GU}$ | 0 | 1 | 0 | DDA$_{CG}$ | 0 | 0 | 1 | 1 |
| | AD$_{AU}$ | 1 | 0 | 0 | AD$_{GU}$ | 1 | 0 | 0 | DAA$_{CG}$ | 0 | 1 | 0 | 0 |
| | AA$_{AU}$ | 1 | 1 | 1 | AA$_{GU}$ | 1 | 1 | 0 | DAO$_{CG}$ | 0 | 1 | 1 | 1 |
| | ADD$_{CG}$ | 1 | 0 | 0 | ADD$_{CG}$ | 1 | 0 | 0 | ADD$_{CG}$ | 1 | 0 | 1 | 1 |
| | ADA$_{CG}$ | 1 | 0 | 1 | ADA$_{CG}$ | 1 | 1 | 0 | ADA$_{CG}$ | 1 | 1 | 0 | 0 |

$a)$ Especially in this case, we defined that if $TS(D_j) = 0 \neq 0$, the output state is $|y'\rangle = |1\rangle|0\rangle$.
is shown (Figure S11, Supporting Information and Table 4). For the RNA-CG nucleotide base pair, although its TS(D) intensity is higher than that of DNA-CG, their truth tables are the same. For the AU nucleotide base pair, when proton \( H_i \) is transferred from the DD$_{AU}$ state to the AD$_{AU}$ state, the NC of adenine (M1) changes from positive to negative (Figure S12, Supporting Information), where an electron is trapped in the adenine group and there is no TS(D)$_i$ peak in the AD$_{AU}$ state. Our results reveal that in the singlet state with phosphate group charges \((-1, -1)\), the truth table of the AU nucleotide base pair satisfies the quantum CNOT or classical XOR or NXOR logic gate; in comparison, the AU nucleotide base pair is a classical logic gate (Table 1). However, for the GU nucleotide base pair, when proton transfer takes place, the planar structure of the base pair is tilted.[54] and TS(D)$_i$/DOS(D)$_i$ is zero. Hence, the GU base pair is not qualified as a quantum logic gate. Essentially, ET in nucleic acids is dominated by the phosphate group and the H bond between the nucleobase pairs.

2.4. ET Mechanism

The TS of the stacked AC and GT nucleobases was calculated, and the results show that the \( \pi\) stacking of the eclipsed and staggered nucleobases allows electrons to pass through the backbone. We have proposed six pathways along the DNA phosphodiester backbone to calculate TS(D)$_i$, and all show distinct peaks (Figure S14, Supporting Information). This finding reveals that the ET pathway along the phosphodiester backbone is due to \( \pi \)-orbital overlap.[55-57] In contrast, the individual deoxyribose and ribose groups are not good conductors (Figure S14, Supporting Information); however, the combination of the ribose (deoxyribose) and phosphate groups is able to conduct electrons. Hence, the H bond between the nucleobase pairs mediates PCET, and the pathway can pass through the intrastrand and interstrand. In this scenario, the ET pathway and PCET mechanisms in DNA and RNA are similar.

2.5. Proteintronics

Notably, both DNA and RNA are potent 2-qubit and 3-qubit logic gates. To develop a 1-qubit logic gate with one H bond, we further explored whether the amino acid pair can fulfill this property. TS calculations were carried out on a pair of two amino acids at the interface of the interpeptide chain, and the proton transfer potential energy curve also elucidated two distinct states (Figure S15, Supporting Information). Interestingly, for a pair of amino acids Glu$_{235}$...Lys$_{91}$ extracted from the protein cytochrome BC1 complex (PDB ID: 1kyo), in the interpeptide chain, ET takes place when the proton HO$_{Glu}$ moves progressively from the AGlu$_{235}$...Lys$_{91}$ state to the D$_{Glu_{235}}$...Lys$_{91}$ state. The truth table indicates that D$_{Glu_{235}}$...Lys$_{91}$ is a Pauli-X gate in the singlet state and is not in the triplet state (Figure S15a1-a4, Supporting Information and Table 5).

However, the TS for a pair of amino acids Ser$_{178}$...Glu$_{184}$ extracted from the interpeptide in the sulfite oxidase (PDB ID: 1ogp) in the triplet state represents TS$_s(D_i) \neq 0$ for the spin-down (\( \beta \)) state and TS$_s(D_i) = 0$ for the spin-up (\( \alpha \)) state, corresponding to the spin-polarized current for the spin-down and spin-up states being \( I_\beta \neq 0 \) and \( I_\alpha = 0 \), respectively (Figure S15b1-b4, Supporting Information and Table 5). As the spin current is defined as \( I_y = I_\alpha - I_\beta \), a negative spin current.[58-59] If we define the input states A$_{Ser_{178}}$...Glu$_{184}$ = \{0\} and D$_{Ser_{178}}$...Glu$_{184}$ = \{1\}, then we have a Pauli-Z gate. Note that because there is no signal at the \{0\} state and a negative spin current at the \{1\} state, the state change is \{0\} \( \rightarrow \) \{0\} and \{1\} \( \rightarrow \) \{1\}. In contrast, if we define D$_{Ser_{178}}$...Glu$_{184}$ = \{0\} and A$_{Ser_{178}}$...Glu$_{184}$ = \{1\} in the reverse way, and by multiplying the imaginary number \( i \) through the algorithm, then the input state \( |\alpha\rangle = |0\rangle \langle 1| \) gives the output state \( |\gamma\rangle = -i |1\rangle \langle 0| \), and it obeys a Pauli-Y gate. Moreover, in the singlet state, Ser$_{178}$...Glu$_{184}$ shows a Pauli-X gate. Hence, the amino acid pair Ser$_{178}$...Glu$_{184}$ can be any one of the Pauli gates.

2.6. Universal Quantum Logic Gate

In accordance, we obtained 3-, 2-, and 1-qubit gates based on DNAtronics, RNAtronics, and proteintronics. Nevertheless, it
is interesting to investigate whether the bionano quantum logic gate that we obtained is universal. A universal quantum logic gate should comprise a Clifford group and a T-phase gate.[66,67] The Clifford group consists of Hadamard, rotation, and CNOT gates.[68] We are able to obtain the Hadamard gate (T), which is a linear combination of Pauli-X (X) and Pauli-Z (Z) gates, \( T = (X + Z)/\sqrt{2} \). As the Pauli-Y gate is similar to the Pauli-Z gate,[63] it is possible to use the 1-qubit amplitude \( c_0|0\rangle + c_1|1\rangle \), where \( (c_0, c_1) = \left( \cos \left( \frac{\pi}{4} \right), \sin \left( \frac{\pi}{4} \right) \right) \) and \( \theta \) and \( \varphi \) are the phase angles, to obtain the rotation gate \( R(\theta) = \sigma_0 \cos \left( \frac{\varphi}{2} \right) - i\sigma_1 \sin \left( \frac{\varphi}{2} \right) \) with \( j = x, y, \) and \( z \), using the Pauli gates.[69] Note that \( \sigma_0 \) and \( \sigma_1 \) are the Pauli operators or Pauli gates. As the phase gate

\[ S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} = \sqrt{Z} = (i + Z)/\sqrt{2} \] and \( T = \sqrt{S} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix} \),

where a self-inverse matrix \( A \) satisfies \( A^2 = I = \) identity matrix and \( \sqrt{A} = (i + A)/\sqrt{2} \) with a given A gate, \( \sqrt{A} \) gate can be obtained.[70] Therefore, the phase gates \( S \) and \( T \) can be built from Pauli gates. Notably, our designated 1-, 2-, and 3-qubit gates fulfill the requirement of a universal quantum logic gate. In advance, CNOT and Toffoli gates could be used in topological QCs.[71] Under these circumstances, complete quantum logic gates could be achieved from nucleic acids and proteins.

2.7. Thermal Effect on ET Signal Transduction

Notably, the nucleotide base pairs can be stabilized by H bonding and \( \pi-\pi \)-stacking interactions. When the two nearest neighboring bases are close enough to allow two 2p-\( \pi \) orbitals to overlap, TS\((D_j) \neq 0 \) (Figure S4, Supporting Information). In contrast, when the 2p-\( \pi \)-orbitals are mismatched due to the base planes sliding or a twisted motion, the TS\((D_j) \) peak disappears. This result indicates that the canonical conditions for the ET pathway along the nucleotide strand are via H-bonding and \( \pi-\pi \)-stacking interactions.

To mimic a large array consisting of nucleotide base pairs, a 24-mer B-DNA sequence was investigated to explore ET signal propagation. Subsequently, we conducted molecular dynamics (MD) simulation to study the fluctuation of the distance between the nucleotide base pairs in the strand and stacking angles, showing pulse signal propagation versus MD time (Figure S16, Supporting Information). For example, in the case of the A\(_3\)–T\(_{20}\) base pair, the pulse output of the H-bond length is 1 when both the distances \( d(N_{n_0} \rightarrow O_4) \) and \( d(N_1 \rightarrow N_{j}) \) are less than their optimized distances; otherwise, it is 0. Similarly, the pulse output of the distance between the stacked nucleobases T\(_{19}\)–T\(_{20}\) is 1 (or 0) at the distance \( d(cm_{T_{19}} \rightarrow cm_{T_{20}}) \) < (or >) 3.5 Å, where \( cm_{T_{19}} \) and \( cm_{T_{20}} \) are the center of mass of the T\(_{19}\) and T\(_{20}\) nucleobases, respectively. As no proton transfer quantum tunneling was involved in MD simulation, this approach was used to examine whether the pulse signal is attributed to thermal motion, leading to the fluctuation of the H bond length in the nucleotide base pair and the distance between the two stacked bases along the strand. These findings also suggest a plausible long-distance ET mechanism and intrinsic signal pattern in nucleic acids. Note that the signal pattern depends on the nucleic acid sequence. Hence, the nucleic acid sequence can be distinguished by measuring the signal pattern.

3. Conclusion and Perspectives

The present study has reported a single-residue pair-transistor technique based on the PCET principle to achieve various quantum logic gates. The uniqueness of this method lies in the modularity of the quantum logic gate. The implemented quantum logic gates achieve a universal QC. Our work provides a practical approach to quantum computation with nanoscale molecular transistors rather than with classical liquid computers.

The advantages of the biomolecule-based logic gates are 1) small sizes of the electronic devices and the ability of extending Moore’s law; 2) low cost, low power consumption, and high efficiency; and 3) ease of construction of the functional logic gates by chemical synthesis.

It is feasible to use biomolecules (DNA, RNA, and protein residue pairs) to conveniently construct subnanoscale molecular transistors and explore the potential of building QCs. Energetically, our quantum chemical computations showed that the total energy of all but one studied residue pair is negative and that they are highly stable. Only GU pair is unstable when the proton is transferred and its structure is tilted. As the proton is confined in the H-bond with a double-well potential, the proton is under controlled conditions.

The feasibility of biomolecular quantum logic gates designed in solid-state devices based on the PCET mechanism is that it neither considers the solution pH effect on biomolecules, nor requires external radiation. According to our computational results, the proton transfer energy barrier is large enough to distinguish the qubit states, |0\rangle and |1\rangle. In vacuum, the qubit system can be described by pure states. However, in solution at finite temperature, the mixed state should be considered and can be described by density matrix. Many studies[67–69] showed that the density matrix is not necessarily unitary and it allows us to use mixed states in QCs by extending Hilbert space to Liouville space. Therefore, the temperature effect on the mixed state can be overcome.

The performance of a qubit is determined by how accurately the operation acts on the qubit and how long its state is retained. It is of particular importance to evaluate the gate fidelity, which depends on the ratio of the gating time to the decoherence time.[70] For example, in the NMR quantum logic gate system, the projection of the final propagation state to the expected state is analyzed to evaluate the accuracy or fidelity in the presence of an external field. Generally, by optimizing the external field, the fidelity can achieve better than 99.9%.[71–75] As the position of the proton is easier to be determined than the electron, the initial state and output state can be detected more precisely.

In his seminal paper,[76] DiVincenzo proposed five criteria for defining the reliability of QCs. We explore these criteria with regard to the subject biomolecule-based device.

1) **A scalable physical system with well-characterized qubits.** Our molecular transistor is an individual logic gate and is suitable for scalable QCs. A QC is composed of a collection of qubits. The entanglement of a set of qubits allows multiple states to act at the same time; in contrast, the classical bits without entanglement have one well-defined value at a time. Therefore, a QC with entanglement can conduct computations much more efficiently. Nowadays, to build a quantum circuit, an entangled state, such as two qubits Bell state, three qubits Greenberger–Horne–Zeilinger state,[77,78] multiqubits entangled
state, etc., has been designed by CNOT and Hadamard gates. Our quantum logic gate is universal (discussed in Section 2.6) and can be used to achieve entangled states.

2) The ability to initialize the state of the qubits to a simple fiducial state. Since the proton position can be identified, as shown in Figure 2, it is possible to initialize the state of the qubits.

3) Long relevant decoherence times, much longer than the gate operation time. The gate operation time is defined as the minimum time of quantum gate operation on qubits and obeys $\tau_{\text{gate}} = \frac{eV}{C_0}$, where $E = E_{\text{g}} + E_{\text{i}}$ is the initial state energy and $E_{\text{g}}$: the target state energy, $\mu = \sqrt{x^2 + (\alpha/E)^2(1 - w^2)}$, $x = E_{\text{g}} - E_{\text{i}}$, and $w = |g(e)|$ is the overlap between the initial state and final state. An underdamped double-well system has a long decoherence time. We here use the decoherence time based on the spin-boson model and $\tau_{\text{decoherence}} = \frac{1}{\alpha} \pi \Delta \cot \left( \frac{\Delta h}{\pi} \right) \sim \alpha \Delta \sim \alpha \Delta_0 \equiv \alpha \omega_0 = \alpha \sqrt{\frac{e}{C_0}}$ in the ohmic region and at low temperature $\cot \left( \frac{\Delta h}{\pi} \right) \approx 1$. Here, $\alpha$ is the coupling constant, $\Delta$ is the renormalized tunneling matrix, $\Delta_0$ is the bare tunneling matrix, $V$ is the second derivative of the proton transfer potential surface at the minimum points, and $m_p$ is the proton mass.

By taking $E_{\text{g}} = 0.00$ kcal mol$^{-1}$, $E_{\text{i}} = 30.00$ kcal mol$^{-1}$ from Figure 2, Supporting Information and $w = 0.01$, where the states, $|0\rangle$ and $|1\rangle$, are well separated and the overlap of wave packets is low. We obtain $\tau_{\text{gate}} = 1.0 \times 10^{-14}$ s. A crude estimation shows that $\tau_{\text{decoherence, underdamp}} = 5.0 \times 10^{-9}$ sec, where $\alpha = 0.01$ in the underdamped regime, however, $\tau_{\text{decoherence, overdamp}} = 1.0 \times 10^{-7}$ sec, where $\alpha = 0.2$ in the overdamped regime. Here $V$ is taken from Figure 2, Supporting Information. As DiVincenzo suggested, for an individual quantum gate with a successful error correction the $\tau_{\text{decoherence}}$ should be $10^4 - 10^5$ times of $\tau_{\text{gate}}$. Our quantum logic gate fully agrees with DiVincenzo's criteria in both overdamped and underdamped regimes.

4) A “universal” set of quantum states. The implementation of complete universal quantum logic gates based on nucleic acids and proteins has been discussed in Section 2.6.

5) A qubit-specific measurement capability. The readout measurement relies on the high-precision detection of the target wave packet. For molecular transistors, it does not require an external field, which is different from ion trap and NMR experiments. Therefore, the fidelity of readout measurement of molecular transistors is high because the techniques can be used to detect the proton position directly and the readout state of qubits.

There are several worthwhile issues for future studies. For example, our molecular transistor could be constructed to conduct quantum circuits. Our qubit could be used as the building block of the lattice in the Kitaev model for Majorana fermion, parafermion, and fracton model which are able to generate pseudoparticles, such as anyons and beyond, and this suggests a fundamental application in topological QCs. In addition, based on the feature of the ET pulse signal pattern along the nucleic acid sequence, the molecular junction technique might be applied to diagnose defects in nucleic acids. We encourage the use of residue pair-based computing elements for nanomedicine applications. Further study of entanglement and dephasing is particularly interesting. One challenge is to explore more molecular transistors that can be used as quantum logic gates in future developments.

4. Experimental Section

All DFT calculations were carried out using the Gaussian 16 program. The system was constructed with a residue-pair transistor wired to two Au electrodes through the tip’s S atoms. Herein, the electrodes, i.e., source and drain, consisted of four layers of Au 3 × 3 lattice along the Au(111) direction, and the tip’s S atom was 2.32 Å from the Au interface. In addition, the geometries of all systems were optimized at the B3LYP level. The basis set used was 6-311++G(d, p) for the C, H, N, O, S, and P atoms, whereas the LANL2DZ basis set was used for the Au atoms. We carried out ab initio quantum calculations to optimize the geometry. An ALACANT program which follows an onion shell structure to construct the device part and the far bulk electrode parts, was used to calculate the TS of ET based on DFT-non-equilibrium green function (NEGF) theory. The general features of the electronic structures of the residue pair and the Au electrodes (the device part) were computed using the DFT local density approximation level with a minimal basis set. A semiempirical tight-binding Bethe lattice model was used for the far bulk electrode parts. The molecular junction denotes the source (left electrode)–residue pair–(right electrode) drain.

According to Landauer’s formula, the conductance for the singlet state, the conductance is given as

$$G = \frac{2e^2}{h} \int_{-\infty}^{\infty} dE \Delta TS(E, V_{\text{bias}} = 0) \left[ \frac{-\partial f(E)}{\partial E} \right]$$

and its relevant current–voltage curve follows

$$I = \frac{2e}{h} \int_{-\infty}^{\infty} dE \Delta TS(E, V_{\text{bias}}) \left[ f_f \left( E + \frac{eV_{\text{bias}}}{2} \right) - f_i \left( E \right) - \frac{eV_{\text{bias}}}{2} \right]$$

where $h$ is Planck’s constant, $e$ is the electric charge, $E$ is the energy, $f(E)$ is the Fermi–Dirac distribution, $TS(E, V_{\text{bias}})$ is the TS, $V_{\text{bias}}$ is the bias voltage, $I_{\text{s}}$ is the charge current, and $I_{\text{f}}(V_f)$ is the Fermi–Dirac distribution for the left (right) electrode. Note that for the singlet state, there is charge current only. Because the Fermi–Dirac distribution is close to a step function and its derivative is a sharp bell-like function centered at the Fermi energy level $E_F$, the conductance and charge current are $TS(E, V_{\text{bias}})$ dependent. We define the $\Delta$ value as the bandgap between the LUMO and the HOMO. When the $\Delta$ value is less than 0.05 eV and the DOS around the $E_F$ covers both the HOMO and LUMO energy levels, a TS peak appears within the range of $D_{\text{TS}} = \left[ \frac{-eV_{\text{bias}}}{2}, \frac{eV_{\text{bias}}}{2} \right]$. Under this circumstance, the delocalized electron density distribution in the molecular junction leads to a tendency for electron tunneling through these systems, i.e., a TS($D_{\text{TS}}$) peak exists. Therefore, the peak indicates a plausible conductance or charge current; otherwise, if TS($D_{\text{TS}}$) is zero, then the electron cannot tunnel through the residue pair.

However, in the case of high spin states, such as triplet and quintet states, the conductance and the current–voltage curve are

$$G_{\sigma} = \frac{e^2}{h} \int_{-\infty}^{\infty} dE \Delta TS_{\sigma}(E, V_{\text{bias}} = 0) \left[ \frac{-\partial f(E)}{\partial E} \right]$$

and

$$I_{\sigma} = \frac{e}{h} \int_{-\infty}^{\infty} dE \Delta TS_{\sigma}(E, V_{\text{bias}}) \left[ f_f \left( E + \frac{eV_{\text{bias}}}{2} \right) - f_i \left( E \right) - \frac{eV_{\text{bias}}}{2} \right]$$

where the subscript $\sigma$ indicates spin up ($\uparrow$) and spin down ($\downarrow$) and $TS_{\sigma}(E, V_{\text{bias}})$ is the TS for the spin $\sigma$. The charge current can be written in terms of $I_{\sigma} = I_{\uparrow} + I_{\downarrow}$, where $I_{\uparrow}(I_{\downarrow})$ is the spin-polarized current and the spin current is $I_{\uparrow} - I_{\downarrow}$.
MD simulations were conducted using the NAMD program[103] and the CHARMM27 force field.[104] The DNA structure was taken from the PDB codes 1bna with 24 base pairs. Na\(^+\) or Cl\(^-\) ions were added to neutralize the system, and the salt molar concentration in solution was set at 0.15 M. Then, the DNA was solvated with TIP4P water molecules in a 70.0 \(\times\) 70.0 \(\times\) 70.0 \(\AA\)\(^3\) cubic box. The particle mesh Ewald algorithm[105] was used to treat the long-range electrostatic interactions, and the SHAKE algorithm[106] was applied to constrain the bonds involving hydrogen atoms. Nonbonding interactions were truncated at 12.0 Å. Then, the solvated system was subjected to heating to 300.0 K, followed by 10.0 ns at equilibrium. Finally, a 10.0 ps MD simulation was conducted for analysis.

Supporting Information
Supporting Information is available from the Wiley Online Library or from the author.

Acknowledgements
S.Y.S and D.Y.Y. contributed equally to this work. S.Y.S. and D.Y.Y. are grateful to the Ministry of Science and Technology in Taiwan for financial support via grants MOST-109-2113-M-010-004 and MOST-109-2113-M-001-023, respectively. The Supporting Information of this article can be found here: https://authorea.com/doi/full/10.22541/au.161462308.84219902/v1.

Conflict of Interest
The authors declare no conflict of interest.

Data Availability Statement
The data that supports the findings of this study are available in the supplementary material of this article.

Keywords
nucleobase pairs, nucleotide base pairs, Pauli gates, quantum logic gates, SWAP gates, Toffoli gates

Received: December 7, 2020
Revised: February 9, 2021
Published online:

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