Stark tuning of the charge states of a two-donor molecule in silicon

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Abstract
A singly ionized two-donor molecule in silicon is an interesting test-bed system for implementing a quantum bit using charge degrees of freedom at the atomic limit of device fabrication. The operating principles of such a device are based on wavefunction symmetries defined by charge localizations and energy gaps in the spectrum. The Stark-shifted electronic structure of a two-donor phosphorus molecule is investigated using a multi-million-atom tight-binding framework. The effects of surface (S) and barrier (B) gates are analyzed for various voltage regimes. It is found that gate control is smooth for any donor separation, although at certain donor orientations the S and B gates may alter in functionality. Effects such as interface ionization, saturation of the lowest energy gap, and sensitivity to donor and gate placements are also investigated. Excited molecular states of P2+ are found to impose limits on the allowed donor separations and operating gate voltages for coherent operation. This work therefore outlines and analyzes the various issues that are of importance in the design and control of such donor molecular systems.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Single-donor systems in silicon have been the subject of much research in recent years due to the promise of long spin coherence times and the expertise of the semiconductor industry in silicon-based nanoscale device fabrication. Quantum computing (QC) proposals using electronic states of single donors have emerged and become popular as a result [1–5]. Recent experiments have not only probed the physics of single donors [6–10], but have also made progress towards precision control and fabrication of few-donor devices [11–18].

Although the initial donor qubit proposals utilized the spin of the donor electron or nucleus to encode qubits [1, 2], one can also envisage fabricating a simple donor molecule in silicon and controlling its charge degrees of freedom. A charge qubit has been proposed as a singly ionized system of two phosphorus donors (P2+) in a matrix of Si atoms [4]. Steps along this direction have been achieved experimentally with charge state transfer between two P donors in silicon [11] and a single electron in a donor-interface double well forming a new hybrid molecular system [6]. Despite possessing the disadvantages of shorter decoherence times, such a charge qubit system is easier to probe experimentally and may help to provide a deeper level of understanding of small donor complexes in silicon [16] and their quantum control using gate fields. The P2+ donor molecule is also more amenable to measurements as the donor electron can be localized to particular impurities by means of appropriate gate placement and voltage pulses. Microwave-driven experiments have already been proposed to investigate the parameter space and physical operation of such devices [28]. Precision placement
of a few donors has also been achieved recently both from STM (bottom-up) [16] and ion-implantation (top-down) fabrication approaches [12, 13], highlighting the urgency for a detailed theoretical study of few-donor level devices.

The $P_2^+$ donor molecule also forms the building blocks of the coherent charge transfer mechanism proposed in [19]. In such a scheme, quantum information encoded in the spin or in the charge of a donor electron can be transported coherently through a chain of ionized donors by an adiabatic pathway realized through voltage pulses applied to electrical gates. Termined as coherent tunneling adiabatic passage (CTAP), this mechanism may provide a robust way to transfer information in a circuit of donor qubits [20, 21].

The Coulomb potential of each donor produces 3D confined states, analogous to quantum dots but on smaller length scales. If two donors are located close-by, their quantum states hybridize and they act as a molecule embedded in a host. The electronic structure of such a molecule is significantly different from an $H_2^+$ molecule in vacuum due to contributions of the momentum space of the host material. Also, it is possible to exercise gate control over each donor and to tune their electronic properties to suit the requirements of the application. An important parameter of interest in a $P_2^+$ molecule for QC applications is the lowest symmetric–antisymmetric energy gap ($\Delta_{S-AS}$). This gap is a function of the detuned energies of the donors and the tunnel coupling between them, both of which can be controlled by external gates. A previous work [22] had utilized effective mass theory (EMT) to show that the inter-donor tunnel coupling suffers from the same sensitivity to relative donor placements as the inter-donor exchange coupling for spin qubits [23]. In [24], the same approach was used to show that the $\Delta_{S-AS}$ can be controlled smoothly by uniform electric fields for both homo- and hetero-polar donor species.

In this work, we employed atomistic tight-binding (TB) theory with a model for P impurities in Si that accurately captures the entire single-donor spectrum and wavefunctions. By solving the full tight-binding Hamiltonian including gate potentials for realistic systems of about 3 million atoms, we are able to obtain any number of states of the $P_2^+$ spectrum. The technique also takes into account the full band structure of Si, an essential feature for studying momentum space effects which are typically ignored in most calculations. Previous works [22, 24] on the $P_2^+$ donor molecule have ignored the effects of the excited manifold on device operations. However, in the presence of significant gate bias, these excited states can disrupt normal device operation by entering the manifold of states used in quantum computing operations. Furthermore, the effects of realistic gate potential profiles with gate-crosstalk on the energy gaps need to be investigated as opposed to the simplistic uniform electric fields generally used. A gate can also cause surface ionization of the bound electron at higher biases, thus limiting the control regime in practice. The presence of nearby interfaces can significantly distort the donor wavefunctions and affect charge qubit operations. Since the previous works concentrated on bulk systems, the above-mentioned design issues that are likely to be encountered in experiments have been neglected.

It is also important to go beyond the EMT assumptions of only the valley minima states contributing to the donor wavefunctions, and to consider a more comprehensive Bloch structure of Si as is done in tight-binding. In the case of inter-qubit exchange coupling for spin qubits, Wellard et al [29] showed that oscillations of the exchange coupling $J(V)$ could be damped to some extent if an extended set of Bloch states is considered rather than the six valley minima states to expand the donor wavefunction. In [29] they also calculated the angular dependence of $J(V)$ for a fixed radial separation of donors and showed that a gate bias was not able to alter $J(V)$ significantly for certain angular separations between donors. It remains to be seen if the $\Delta_{S-AS}$ also suffers from this controllability problem.

As experiments are getting closer to fabricating few-donor devices [11], it is important to develop a detailed theoretical model that analyzes the various aspects of qubit control and design space. While the gate geometries and the associated electrostatics may vary from one experiment to another, our goal is to establish a comprehensive numerical framework that can be easily tuned to model specific experiments. However, the various features and operating regimes elucidated in this work are likely to be observed for large enough voltage sweeps. This TB approach has been highly successful in modeling and interpreting recent donor experiments [6, 8, 26].

This paper is organized into three parts. In section 2, the geometry of a P-donor-based charge qubit in Si is described and the various control parameters studied here are outlined. In section 3, the details of the tight-binding method is described. Section 4 presents the results and discusses the controllability issues in detail.

2. $P_2^+$ donor device geometry

A schematic of a $P_2^+$ donor molecular device in Si is illustrated in figure 1. The P donors are separated by a distance $R$ nm and an angle $\Theta$ measured from the [100] axis in a plane parallel to the oxide. A barrier gate (B-gate) is placed midway between the impurities and controls the potential barrier between them. A surface gate (S-gate) is placed a distance $L_S$ (measured with respect to the center of the S gate) away from the left impurity and controls the detuning of the impurity states. The oxide thickness $T_{ox}$ is 5 nm, while the gate lengths are 10 nm. The impurities are buried at a depth $D_V$ below the oxide and a distance $D_h$ from the lateral interfaces.

It was shown in a previous work [30] that a donor at the center of a 30 nm cubic box subjected to a hard-wall boundary condition can essentially be treated as a bulk donor in this model. Any increase in domain size affects the lowest manifold of s-states by less than 0.1 $\mu$eV, which is sufficiently small compared to the meV energy scale of the donor states. This consideration was taken into account while choosing simulation domains in cases where boundary effects are to be neglected.

The gates are of rectangular shape, and are assumed to be infinite in the [001] direction, as are in typical experiments. This means that the gate potential is constant in the [001] direction. The symmetry of the device ensures
that all the calculated quantities are independent of the [001] direction, except for the effects of donor displacements in [001], which are investigated in figure 7. The semiclassical TCAD simulations have been done on a much larger device assuming a grounded back gate. The detailed device geometry, parameters and the TCAD solutions can be found in [29, 31]. The tight-binding-based quantum mechanical electron structure calculations are then performed on the relevant portions of the device. Typical TB simulations are on dimensions of 50 nm × 40 nm × 30 nm. Wherever possible, we have chosen the smallest device volumes to minimize computation times while making sure that the results are not affected by finite lateral boundaries.

First, we study the molecular spectrum of the system without any gate voltage, taking into account the complicated band structure of Si. Then we investigate how this spectrum, and in particular the \( \Delta_{S\rightarrow AS} \), can be controlled by surface and barrier gates. Effects of design parameters such as \( L_S \), \( D_V \), \( R_t \), \( \Theta \), \( V_S \) and \( V_B \) are also explored. In particular, the energy gaps \( \Delta_{12} \) and \( \Delta_{23} \) are studied. \( \Delta_{12} \) represents the energy difference between the first excited state (\( S_2 \)) and the ground state (\( S_1 \)), while \( \Delta_{23} \) represents the energy difference between the second excited state (\( S_3 \)) and the first (\( S_1 \)).

3. Tight-binding solution of the solid-state donor molecular system

The semi-empirical TB method [33] employed here utilizes the 20-band \( sp^3d^5s^* \) nearest-neighbor model. The Hamiltonian is expressed in real space with a basis of localized atomic orbitals. The 20-band TB parameters for Si are optimized by genetic algorithms [34, 35] to reproduce the bulk band structure of the host. Once a set of such parameters is found, it can be used for atomistic modeling of a generic device made of the host. A single P impurity is represented by a Coulomb potential screened by the dielectric constant of Si (\( \epsilon_{Si} \)) and subjected to a cutoff potential \( U_0 \) at the impurity site. This core correcting potential \( U_0 \) is adjusted to reproduce the single-donor ground state binding energy. The total TB Hamiltonian is of the form

\[
H = H_0 + e V_{Di} + e V_{D2} + \frac{e^2}{4\pi \epsilon_{Si} |R_1 - R_2|} + e V_G(S, V_B) \quad (1)
\]

where the first term is the crystal Hamiltonian of Si, the second and third terms the potential energy due to the two donor nuclei, the fourth term the nuclear repulsion of the two positively charged impurity cores and the last term the potential energy due to the surface and barrier gates obtained from a commercial Poisson solver [32]. The single-impurity potential is expressed as

\[
V_{Di}(r) = -\frac{e}{4\pi \epsilon_{Si} |r - R_i|}, \quad r \neq R_i \quad (2)
\]

\[
V_{Di}(r) = -U_0, \quad r = R_i \quad (3)
\]

where \( R_i \) is the location of the \( i \)th impurity. Interfaces are treated by closed boundary conditions with a model of surface passivation of dangling bonds [36]. The full atomistic Hamiltonian of about 3 million Si atoms was solved by a parallel Lanczos/Block Lanczos algorithm to obtain the eigenvalues and wavefunctions in the desired energy range [35]. Each data point in this work required about 6 h on 48 processors.\(^5\)

The tight-binding method used here is under the hood of the Nanoelectronic Modeling Tool (NEMO-3D) [35, 37] and had been successfully used to verify the Stark shift of the hyperfine coupling between a donor and its nucleus [26], in good agreement with experiments [8] and with momentum space methods [25]. The same method was also applied to investigate the orbital Stark shift of a donor-interface well system, and was verified with single-donor transport experiments in FinFETs [6].

4. Results and discussions

4.1. The molecular spectrum of \( P_{2+} \) at zero gate bias

The lowest six states of a single group V donor in Si are of 1s type due to the sixfold-degenerate conduction band minima of Si. The sharp confining potential in the vicinity of the donor nucleus causes coupling between orbital states in different conduction band valleys, a phenomena termed as valley–orbit (VO) coupling. The net effect of the VO interaction is a splitting of the six 1s orbital states into a singlet (\( A_1 \)), a triplet (\( T_2 \)) and a doublet (\( E_1 \)) orbital manifolds. The strength of this VO interaction varies from one donor species to another, and is caused by a number of microscopic properties such as variation of the dielectric constant of Si from its bulk value, local strain originating from bonds between the donor and the Si atoms, to name a few. For an isolated P donor in Si, the (\( A_1 \)), (\( T_2 \)) and (\( E_1 \)) states are bound at \(-45.6, -33.9 \) and \(-32.6 \) meV, respectively [27]. When two hydrogenic donors are placed near each other, each pair of corresponding 1s states gives rise to a bonding (symmetric) and an anti-bonding (antisymmetric) state.

Figure 2 shows the variation of the binding energies of the 12 lowest molecular states of the \( P_{2+} \) system as a function of donor separation. The binding energies show smooth exponential decay with donor separation \( R \) for donors

\(^5\) nanoHUB.org computational resource of a 256-node 3.3 GHz Pentium Irwindale PC cluster was used. The tight-binding calculations were done with the NEMO-3D tool.
separated along [100] (figure 2(a)), but exhibit some oscillatory behavior for donors separated along [110] (figure 2(b)), consistent with EMT descriptions [22]. For large enough \( R \), the bonding and anti-bonding pairs become almost degenerate and the binding energies reduce to the single P binding energies with double degeneracies. At small \( R \), the bonding state arising from the \( T_2 \) states of each donor approaches the anti-bonding state arising from \( A_1 \) states, causing \( \Delta_{12} \) to be comparable in magnitude to \( \Delta_{12} \). This situation is undesirable in quantum computer architectures since the qubit Hilbert space, which usually consists of the two lowest eigenstates, needs to be well isolated in energy from the rest of the manifold in order to minimize decoherence and errors during operation. In this paper, we will use \( \Delta_{12} = \Delta_{23} \) as a reference level for device operation. If \( \Delta_{12} > \Delta_{23} \), the device is in an undesirable operation regime. Figures 2(c) and (d) show the \( \Delta_{12} \) and \( \Delta_{23} \) energy gaps. It is observed that the donor separations need to be at least about 7 nm for such coherent applications.

4.2. Surface gate control

The function of a surface gate is to provide a potential difference between the two impurities, and hence to control the energy spacing of the eigenstates of one impurity relative to the other. In the device geometry shown in figure 1, a positive bias to the surface gate lowers the energy states of the left impurity relative to the right impurity. The \( A_1 \) state of the left donor moves further below that of the right donor and this increases \( \Delta_{12} \). The \( T_2 \) state of the left donor moves closer to the \( A_1 \) state of the right, which decreases \( \Delta_{23} \). Figures 3(a) and (b) show the variation of \( \Delta_{12} \) and \( \Delta_{23} \), respectively, with an S-gate voltage for three different donor separations along [100]. For larger impurity separations, the slopes of the \( \Delta_{12} \) and \( \Delta_{23} \) curves are steeper. If the impurity separations are larger, then the left impurity experiences a stronger S-gate potential than the right impurity. Hence the detuning is stronger. If the impurities are closer, then the same surface gate voltage provides less potential drop between the two impurities and the surface gate response is weaker.

To elucidate the different voltage regimes shown in figure 3, it is helpful to look at the first three eigenstates of the whole device (top three rows of figure 4) along with the net electrostatic potential profile the device is operating under (second row from the bottom of figure 4). Each column in figure 4 illustrates a snapshot of the donor molecule for a specific surface gate voltage with two donors separated by 15.2 nm along [100] (points marked by the green square data points in figure 3).

At \( V_S = 0 \) (column 3 from left), the two-donor wells are aligned in energy, giving rise to bonding and anti-bonding pairs. The lowest two states (\( S_1 \) & \( S_2 \)) are formed from the symmetric and antisymmetric superpositions of the \( A_1 \) state of each donor. \( S_3 \) is a bonding state arising from the \( T_2 \) states.

As \( V_S \) is increased up to 0.2 V (column 4), the device is in the linear operation regime shown in figure 3. The left impurity is lower in energy than the right, giving rise to a left localized ground state (\( A_1 \) of left P) and a right localized first excited state (\( A_1 \) of right P), while state three arises from the \( T_2 \) state of the left donor. A plot of the total potential shows that the
Figure 3. Effect of surface gate bias on (a) $\Delta_{12}$ and (b) $\Delta_{23}$ for three different donor separations. The surface gate is located 10.8 nm ($L_s$) from the left donor, while the donors are buried 20.1 nm ($D_v$) below the oxide. The B gate is set to ground.

Figure 4. The three lowest electronic states of the donor molecule at various surface gate voltages shown as 2D cuts (in the $xy$ plane). Each column represents the device at a specific voltage. The bottom two rows show the net electrostatic potential (in V) and electric field (in V nm$^{-1}$) in the device, respectively. The electric field is calculated using the relation $\vec{E} = -\vec{V}$. The magnitude $F(x, y) = \sqrt{F_x^2 + F_y^2 + F_z^2}$ is plotted on a log$_{10}$ scale. The top three rows show the first three wavefunction probability amplitudes. The states are labeled as $S_1$, $S_2$ and $S_3$, from more strongly bound to less ($S_1$ being the ground state).
surface gate expands the potential contours of the left impurity relative to the right.

If the S-gate voltage is reversed in polarity to $-0.2$ V (column 2), the effects described above are reversed between the two impurities, with a right localized state appearing as the ground state.

At $V_S = 0.5$ V (column 5), a surface well is formed near the gate and quantum states begin to appear in this well. In a finite-sized nanostructure such as this device, whether the lowest states are at the surface or at the donor is determined by which well is lower in energy. At $V_S = 0.5$ V, the surface well is almost as deep as the donor well. While the ground state of the system is still seen to occur in the left donor, the higher states occur in the surface well. A small increase in bias at this point moves the interface well deeper than the donor well and produces ionization of the donor electron. For a donor close to the surface, the donor well can strongly couple to the interface well and gives rise to the prospect of adiabatic ionization [6, 38–43]. The gate-confined surface states are closely spaced in energy compared to the donor states due to a reduced VO interaction at the interface well. Both $\Delta_{12}$ and $\Delta_{23}$ show a sharp decrease at the onset of this ionization process, as shown in figure 3.

At $V_S = -0.5$ V (column 1), the interface well is raised in energy and does not play a role. The gate voltage is high enough to push the $T_2$ states of the right donor below the $A_1$ state of the left donor. When this happens, any subsequent change of the gate bias causes only a small change in $\Delta_{12}$, and it flattens out, as shown in figure 3(a) for the $R = 15.2$ and $20.1$ nm curves. This is expected as $\Delta_{12}$ is now equal to the splitting between the $A_1$ and $T_2$ of the same donor and has a much weaker field response. The $\Delta_{23}$ curve captures the energy gap between the higher states of the same donor and tends to flatten out also. The energy gaps therefore saturate in this voltage regime.

Since $\Delta_{12}$ is to be less than $\Delta_{23}$ for the donor device, the linear regimes about $V_S = 0$ are important for coherent operations. The operational basis can be either the left and right localized states at modest bias (linear regime), or the bonding and anti-bonding states near zero bias [4]. The ionization regime at high positive bias can be important if the donor electron is to be shuttled from one donor to another by transport along the interface [3] or if a measurement at the surface is to be performed [38].

4.3. Barrier gate control

In contrast to a surface gate, a barrier gate subjects both donors to a similar potential. A positive barrier gate lowers the potential in the region between the two impurities and increases hybridization of the left and right donor states. $\Delta_{12}$ and $\Delta_{23}$ are affected less by B gates than S gates, as exhibited by the smaller slopes (vertical axis voltage scale) of the $\Delta_{12}$–$V_B$ curves of figure 5 compared to those of figure 3. The B gate also generates an interface well which eventually ionizes the donors at high enough gate bias, causing a sharp fall in $\Delta_{12}$ and $\Delta_{23}$, observed around $V_B = 0.5$ V. Figure 6 shows how $\Delta_{12}$ is affected when both S-gate and B-gate biases are present simultaneously. In each curve, the B gate is held fixed at some voltage and the S gate is varied over a range of $-0.5$–$0.5$ V. It was shown in figure 3 that at zero B-gate bias, the $\Delta_{12}$–$V_S$ curve shows a minimum at $V_S = 0$. In the presence of a positive (negative) B-gate bias, this minimum shifts to a negative (positive) $V_S$ value. Since a positive B gate lowers the potential in the barrier regions and binds the electron more tightly between the donors,
\[ \Delta S \text{--AS} (\Delta_{12}) \] increases. Although a negative S-gate bias causes detuning of the two impurities, it also lowers the potential in the barrier region, and thus compensates for the positive barrier gate. Hence, to obtain the same zero-field \( \Delta S \text{--AS} \), a negative S-gate bias is needed, which explains the shift of the \( \Delta_{12} \)-\( V_B \) curve towards a negative \( V_S \) when \( V_B \) is held positive.

Since the gates are separated by only 15 nm in this case, there is significant cross-talk between them. A positive S gate therefore makes the surface well near B gate deeper, and vice versa. As a result the ionization regime shifts to the left with increasing B-gate bias.

Simultaneous S-and B-gate biases can be used to initialize the donor molecule system. At first, each donor has one electron bound to it. To form a \( P_2^+ \) molecule, one electron has to be removed. This can be done by holding \( V_B \) negative so as to raise the barrier between the left and right donors, while applying a simultaneous positive bias to the S gate to ionize the left donor electron to the surface well.

4.4. Sensitivity to donor placement

In this section, we investigate the sensitivity of \( \Delta S \text{--AS} \) to relative donor placements along different directions. In figure 7, the radial separation between the donors is held fixed at 10.8 nm, while the angular separation is varied from 0° to 45° at a fixed donor depth of 20.1 nm. \( \Delta_{12} \) and \( \Delta_{23} \) are plotted in figures 7(a) and (b), respectively, for three different gate configurations.

Although \( \Delta S \text{--AS} \) shows some oscillatory behavior with angular separation, both a barrier and a surface gate voltage are each able to change it significantly. This shows that there is enough gate controllability irrespective of how the donors are placed relative to each other. As a note of comparison, a similar study was done on the two-donor exchange coupling \( J(V) \) in [29]. In contrast to the result obtained here, the \( J(V) \) curve exhibited some gate controllability issues. For certain angular separations between the donors, a gate voltage was not able to alter the magnitude of \( J(V) \) significantly. The absence of such controllability issues in this case is quite encouraging.

While figures 3 and 5 demonstrated smooth gate control over donors separated along [100], figure 8 demonstrates that such smooth control also exists for donors separated along other directions. In addition, figure 8 also demonstrates some geometry effects that need to be considered in practical devices. Figure 8(a) shows the effect of an S gate on \( \Delta_{12} \) for donors separated along three different directions, while figure 8(b) shows the same for a B gate.

The striking feature of the curves is the asymmetry in voltage control between the [111] separation and the other two directions. If both impurities are not on the same \( xz \) plane (figure 1), which happens for [111] separation, then a B gate may subject one donor to a higher potential than the other.
This is more pronounced if the donor depths below the gate are unequal by more than tens of lattice constants. In such a case, a B gate can act as an S gate, and the voltage response curve $\Delta_{12} - V_S$ can show a significantly larger response. The $\Delta_{12} - V_S$ curve of figure 8(b) has a steeper slope for [111] donor separations compared to the [100] and [110] separations.

Similarly, for [111] donor separations, an S gate may be almost equidistant from the two donors and can act as a B gate, thus reducing the voltage response of $\Delta_{12}$ significantly. This is evident by the smaller slope of the [111] curve of figure 8(a) compared to the other two curves. For the device structure considered here with donor separations along [111], the radial distances between the S-gate center and the left and right donors were 26.7 nm and 25.1 nm, respectively. This shows that donor depth below the gate is an important feature in experimental design as surface gates can act as barrier gates and vice versa for certain donor orientations.

4.5. Design issues: gate placement and donor depth

Figure 9(a) shows the effect of varying the distance between the S gate and the left impurity for two donors separated by 15.2 nm along [100]. The slope of the $\Delta_{12} - V_S$ curve is sensitive to $L_S$ because it determines the potential contours the two impurities reside on. It is seen that the slopes of the curves are the steepest when $L_S$ is between 10.8 and 20.1 nm, suggesting that there may be an optimal gate distance for the design purposes. A small $L_S$ of 0 or 5.5 nm is likely to subject both impurities to a strong potential. As a result, the detuning is less responsive.

In figure 9(b), we show how the S-gate response of $\Delta_{12}$ is modified for two different donor depths below the oxide. For both donors at a shallower depth of 10.8 nm, the $\Delta_{12} - V_S$ curve is steeper because proximity of the donors to the gate lends more control. The curve is also seen to flatten off before reaching the ionization regime. This is because the stronger potential brings the $T_2$ state of the left impurity below the $A_1$ state of the right, and causes $\Delta_{12}$ to become saturated before ionization is reached. Any further increase in $V_S$ after 0.2 V, simply captures the energy gap between the $A_1$ and $T_2$ states of the left impurity. In contrast, the curve for 20.1 nm depth reaches ionization directly after the linear regime.

5. Conclusion

Gate control of a $P_2+$ molecular system was investigated in detail from an atomistic tight-binding approach. It was found that excited states can impose limits on the range of operating voltages and donor separations. This arises from the necessity that the qubit Hilbert space needs to be sufficiently isolated from the other states of the system for robust coherent operation. TCAD gate potentials were used to demonstrate that smooth controllability exists over the molecular states of the donors. The detuning of two donors by a surface gate in various voltage regimes was analyzed. It was also shown that the energy gaps are more sensitive to the S gate over B gate, with the exception of certain donor orientations for which the S gate can act like a B gate and vice versa. Simultaneous operation with both S and B gates was shown to shift the minimum energy gap to non-zero gate configurations. Practical control of such a system is also limited by interface ionization, and voltage regimes were established where this could take place. Sensitivity of the energy gaps to donor placement was also investigated. Although the lowest energy gap exhibits oscillatory behavior with donor separations in certain directions, it was found that a gate voltage was always able to magnify it significantly. This confirms that the tunnel-coupling-induced symmetric–antisymmetric energy gap is free from the voltage controllability issue shown in exchange-based donor qubits [29].

The purpose of this work was to highlight the controllability and design issues that an experimental implementation and control of a $P_2+$ molecular system would involve. The focus here has been both on the physical trends and on the quantitative description of some quantities that are of interest in experiments. This $P_2+$ molecule forms the building blocks of structures that can utilize CTAP to transport information across qubits. Realization of CTAP in an actual donor array is likely to involve very precise gate control over quantum states of coupled donors. Detailed understanding of the $P_2+$ system is a prerequisite to understanding more complex CTAP-like structures.

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