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RAPID COMMUNICATION

First-principles calculations on strain tunable hyperfine Stark shift of shallow donors in Si

Zi-Kai Zhou(周子凯)[1] and Jun Kang(康俊)[1,2,†]

[1] *Beijing Computational Science Research Center, Beijing* 100193, *China*
[2] *Department of Physics, Beijing Normal University, Beijing* 100875, *China*

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Control of hyperfine interaction strength of shallow donors in Si is one of the central issues in realizing Kane quantum computers. First-principles calculations on the hyperfine Stark shift of shallow donors are challenging since large supercells are needed to accommodate the delocalized donor wave functions. In this work, we investigated the hyperfine Stark shift and its strain tunability for shallow donors P and As in Si using the potential patching method based on first-principles density functional theory calculations. The good agreement between our calculations and experimental results confirms that the potential patching method is a feasible and accurate first-principles approach for studying wave-function-related properties of shallow impurities, such as the Stark shift parameter. It is further shown that the application of strain expands the range of hyperfine Stark shift and helps improve the response of shallow donor based qubit gates. The results could be useful for developing quantum computing architectures based on shallow donors in Si.

Keywords: shallow donors, first-principles calculations, hyperfine interaction

PACS: 71.15.Mb, 71.55.–i, 31.30.Gs

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1. Introduction

Shallow donors in Si serve as quantum qubits in the Kane proposal for a quantum computing architecture.[1,2] They have long coherence times[3] and are potentially compatible with existing microelectronics. In the Kane proposal, information is encoded by nuclear spins which can be manipulated and measured by tuning the hyperfine coupling between the electron wave function and nucleus.[1,4,5] Therefore, precise control of the donor hyperfine interaction strength is one of the central issues in realizing Kane quantum computers. Such a control can be realized by applying an electric field which leads to a modification of the hyperfine interaction through the Stark effect,[6–8] known as the hyperfine Stark shift. In addition, strain may be further utilized to control the hyperfine Stark shift,[9–11] leading to improved qubit gate speeds and fidelities,[12] and suppressed exchange coupling oscillation.[13,14]

Theoretical modeling of the hyperfine Stark shift and its strain tunability of shallow donors in Si could be helpful for the development of the Kane quantum computer. The key challenge is to accurately describe the donor electron wave function, which extends across thousands of unit cells, under the influence of an electric field and/or strain. The donor hyperfine Stark shift in Si has been broadly investigated by effective mass theory[8,15] and tight-binding methods,[12,16,17] which can yield good agreements with experiments. However, these methods rely heavily on empirical parameters, and their predictive power becomes quite limited when reliable parameters are missing. First-principles calculations based on the density functional theory (DFT) do not suffer from this issue, and naturally include valley repopulation and structural relaxation induced by donors in Si. Nevertheless, conventional DFT calculations are computationally demanding, and their costs scale cubically with system sizes, making it difficult to accurately model shallow donors with delocalized wave functions. There have been several DFT studies that accurately reproduce zero-field hyperfine interactions of donors in Si employing either the Green's function[9,18] or extrapolation methods.[19,20] While the wave function can be well described in the vicinity of the donor site containing a small amount of atoms, full information of the delocalized donor wave function is not available in these approaches, making it difficult to calculate the Stark shift.

Recently, a potential patching method based on first-principles DFT calculations for modeling shallow impurities in semiconductors has been proposed.[21–23] It allows the simulations of large supercells with over 10^4 atoms and yields accurate shallow impurity binding energies. Complete wave functions of the impurity states can also be obtained using this method. However, the applicability of the potential patching method to the calculations of hyperfine interactions has not been investigated yet. In this work, we use the potential patching method to study the strain tunability of the hyperfine Stark

[†]Corresponding author. E-mail: jkang@csrc.ac.cn

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shift of shallow donors P and As in Si. We demonstrate that the method is a feasible approach with a high accuracy to study the wave-function-related properties of shallow impurities such as the Stark shift parameter. It is further shown that the application of strain can help improve the response of shallow donor based qubit gates. The results could be useful for developing Kane quantum computers.

2. Methods

To study shallow donors in Si, we employed the potential patching method[21–23] based on first-principles DFT calculations, which enables simulations with extremely large supercells, ensuring convergence of impurity energy levels and wave functions. Since the structural relaxation before and after the ionization of a shallow impurity is typically negligible, the binding energy of a donor impurity state can be obtained as $E_b = E_{\rm bulk}^{\rm CBM} - E_{\rm im}$, where $E_{\rm im}$ represents the quasiparticle energy of the impurity state, and $E_{\rm bulk}^{\rm CBM}$ corresponds to the conduction band maximum (CBM) energy of the pristine bulk material. Within the Kohn–Sham DFT framework with nonlocal pseudopotentals, $E_{\rm im}$ satisfies the equation

$$\left(-\frac{\nabla^2}{2} + V_{\rm im}(\boldsymbol{r}) + \hat{V}_{\rm NL}\right)\psi_{\rm im} = E_{\rm im}\psi_{\rm im}, \tag{1}$$

where $\psi_{\rm im}$ denotes the impurity wave function, $V_{\rm im}(\boldsymbol{r})$ is the local potential (including ionic, Hartree, and exchange–correlation contributions), and $\hat{V}_{\rm NL}$ represents the nonlocal component of the pseudopotential. Here, a key challenge for DFT calculations is determining $V_{\rm im}(\boldsymbol{r})$ in a large supercell. Conventional self-consistent calculations are not feasible due to the cubic scaling of computational cost. The potential patching method addresses this issue in a divide-and-conquer manner: the local potential in the vicinity of the impurity is extracted from a small supercell calculation, while regions further from the impurity are approximated using the bulk potential plus a Coulomb tail. In this way, the $V_{\rm im}(\boldsymbol{r})$ can be constructed without doing self-consistent calculations. We first compute the local potential $V_{\rm im}^{\rm SC}(\boldsymbol{r})$ within a small supercell $\Omega_{\rm SC}$ containing a charged impurity (in this work, a $+1$ charged 512-atom supercell is used for donors), along with the bulk potential $V_{\rm bulk}(\boldsymbol{r})$ obtained from a pristine host calculation. The potential $V_{\rm im}(\boldsymbol{r})$ felt by electrons in a larger supercell is then approximated as

$$V_{\rm im}(\boldsymbol{r}) = \begin{cases} V_{\rm im}^{\rm SC}(\boldsymbol{r}) - V_{\rm C}(\boldsymbol{r}) + V_{\rm align}, & \boldsymbol{r} \in \Omega_{\rm SC}, \\ V_{\rm bulk}(\boldsymbol{r}) - 1/(\varepsilon r), & \boldsymbol{r} \notin \Omega_{\rm SC}, \end{cases} \tag{2}$$

where ε is the dielectric constant of the host material, taken to be 12.34 for Si.[22] The term $V_{\rm C}(\boldsymbol{r})$ accounts for the Coulomb interaction from periodic images of $\Omega_{\rm SC}$, which is artificial and should be removed from $V_{\rm im}^{\rm SC}(\boldsymbol{r})$. It is given by

$$V_{\rm C}(\boldsymbol{r}) = \sum_{(i,j,k)\neq(0,0,0)} \frac{-1}{\varepsilon|\boldsymbol{r} - (i\boldsymbol{L}_1 + j\boldsymbol{L}_2 + k\boldsymbol{L}_3)|}, \tag{3}$$

where $\boldsymbol{L}_{1,2,3}$ are the supercell lattice vectors. The term $V_{\rm align}$ ensures smooth potential alignment between the interior and exterior of $\Omega_{\rm SC}$. Ideally, with the removal of $V_{\rm C}(\boldsymbol{r})$, the difference between the constructed $V_{\rm im}(\boldsymbol{r})$ and $V_{\rm bulk}(\boldsymbol{r})$ should match the $1/(\varepsilon r)$ tail at the cell boundary of $\Omega_{\rm SC}$. This is indeed the case in our calculations, as seen in Fig. 1 where the atomic site potential difference between the P-doped and pristine Si as a function of distance from the P atom is plotted. Once $V_{\rm im}(\boldsymbol{r})$ is constructed, equation (1) is solved using the folded spectrum method,[24] which allows efficient computation of a few eigenstates within a targeted energy window. This avoids solving for states far from the impurity states of interest, leading to linear-scaling computational costs.

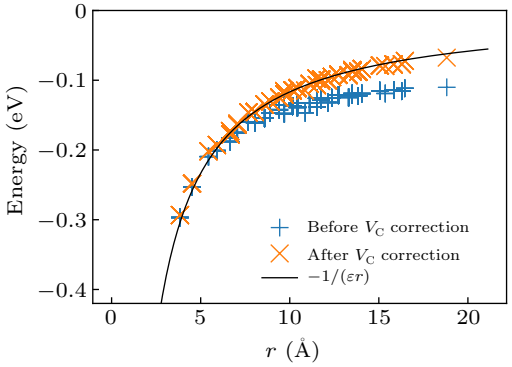


Fig. 1. The atomic site potential difference between the P-doped and pristine Si as a function of distance from the P atom before and after the $V_{\rm C}$ correction.

In practice, $V_{\rm im}^{\rm SC}(\boldsymbol{r})$ is obtained using local or semilocal exchange–correlation functionals. Here we adopted the local density approximation (LDA).[25] To mitigate the self-interaction errors associated with LDA in predicting quasiparticle energies, we first performed Heyd–Scuseria–Ernzerhof (HSE06) hybrid functional[26] calculations for the small supercell $\Omega_{\rm SC}$. Then we applied a correction to the nonlocal pseudopotentials $\hat{V}_{\rm NL}$ of the Si atoms within the first to third nearest neighbor shells of the donor to reproduce the relative energy shift of the donor states due to HSE06. Subsequently, these modified pseudopotentials are employed in large-scale systems. More details about this correction scheme are described in Ref. [23].

All DFT calculations in this work were performed using the PWmat code.[27,28] The plane-wave energy cutoff was set to 18 Ry. The Troullier–Martins norm-conserving pseudopotentials[29] were adopted. The atomic positions were relaxed with the LDA functional until the force on each atom was smaller than 0.01 eV/Å. A single Γ was used for supercell calculations.

3. Results and discussion

The lowest conduction band of Si has six equivalent minima located at about 86% of the way along the $\Gamma \to X$ directions. When a Si atom is substituted by a donor impurity, the

original O_h symmetry is reduced to T_d symmetry. The six-fold valley degeneracy is thus lifted, resulting in three donor states: the singlet A_1 state (the ground state), the triplet T_2 state, and the doublet E state.[30] Figure 2(a) shows the calculated donor binding energies E_b of these states for P and As using the potential patching method with different supercell sizes. Here we considered cubic supercells with length L ranging from $8a$ to $40a$ (a is the lattice constant of Si), containing 4096 to 512000 atoms, respectively. For all the levels, the calculated E_b decreases as the supercell size increases because the donor wave functions are less confined in larger supercells. For the A_1 ground state, good convergence of E_b is achieved when L is larger than $24a$. For the higher T_2 and E states, $L = 32a$ is needed to converge the E_b. The results suggest that to accommodate the shallow donor wave functions in Si from periodic images, one should use supercells with over 10^5 atoms. In Fig. 2(b), the charge densities (namely, the wave function square) of the P donor states in the supercell with $L = 32a$ are presented. With this supercell size the charge is indeed well isolated. Therefore, all subsequent calculations in this work are based on this $L = 32a$ supercell configuration. Table 1 compares the calculated and experimental E_b, and we find excellent agreement for both P and As donors. The maximum error is less than 4 meV, indicating a good accuracy of the potential patching method.

Table 1. The calculated donor binding energies E_b using the $L = 32a$ supercell compared with experiments.[31]

		E_b (meV)		
		A_1	T_2	E
P	Cal.	47.66	34.07	32.40
	Expt.	45.59	33.89	32.58
As	Cal.	57.74	32.83	31.31
	Expt.	53.76	32.67	31.26

For quantum computing architectures based on shallow donors in Si, the control of hyperfine interaction is a central issue. At zero field, the hyperfine interaction strength $A(0)$ is proportional to the wave function square $|\psi(r_0)|^2$ at the donor site r_0.[12] Note that only the A_1 state contributes to $A(0)$ since the wave functions of the T_2 and E states at the donor site are zero. When an electric field $\boldsymbol{E}$ is applied, the wave function can be pulled off the donor site via the Stark effect, and the hyperfine interaction strength $A(\boldsymbol{E})$ differs from $A(0)$. The change $\Delta A(\boldsymbol{E}) = A(\boldsymbol{E}) - A(0)$ can be described by a quadratic dependence[8]

$$\frac{\Delta A(\boldsymbol{E})}{A(0)} = \frac{|\psi(\boldsymbol{E};r_0)|^2}{|\psi(0;r_0)|^2} - 1 = \eta_2 |\boldsymbol{E}|^2, \tag{4}$$

where η_2 is defined as the Stark shift parameter. To determine the η_2, we calculated the $|\psi(\boldsymbol{E};r_0)|^2$ of the A_1 state at the donor site under different electric field strength from 0 to 0.5 V·μm^{-1}, and η_2 was obtained by fitting $\Delta A(\boldsymbol{E})/A(0)$ with a quadratic function of $|\boldsymbol{E}|$. In our calculations, the electric field was introduced by a sawtooth potential with zero mean value. As the wave function of the A_1 state is well isolated [see Fig. 2(b)], the potential jump at the supercell boundary will not cause artificial perturbation. The $\Delta A(\boldsymbol{E})/A(0)$ as a function of $|\boldsymbol{E}|$ is shown. With increasing field strength, $\Delta A(\boldsymbol{E})/A(0)$ decreases due to the Stark effect. The data can be well fitted with quadratic functions. The calculated η_2 is -2.2×10^{-3} μm$^2 \cdot$V^{-2} for P and -0.9×10^{-3} μm$^2 \cdot$V^{-2} for As, which are in good agreement with experimental values of $-(2.5 \pm 0.9) \times 10^{-3}$ μm$^2 \cdot$V^{-1} for P and $-(1.2 \pm 0.3) \times 10^{-3}$ μm$^2 \cdot$V^{-2} for As.[8] The smaller η_2 of As than P can be understood by the larger binding energy of its A_1 state. The results thus validate the capability of the potential patching method to study wave function related properties of shallow impurities in semiconductors.

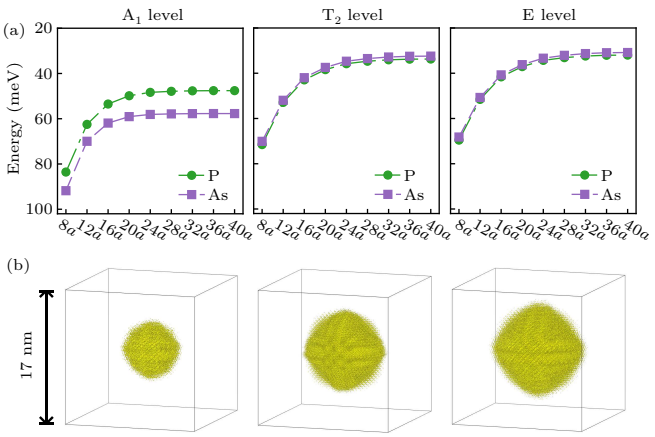


Fig. 2. (a) The calculated donor binding energies E_b of P and As using the potential patching method with different supercell sizes. (b) The charge densities of the P donor states in the supercell with $L = 32a$. The isosurface includes 80% of the total charge.

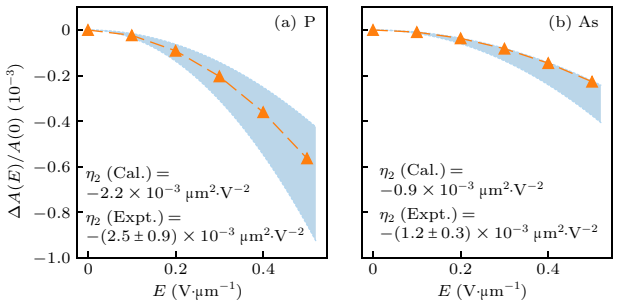


Fig. 3. The $\Delta A(\boldsymbol{E})/A(0)$ as a function of $|\boldsymbol{E}|$ is shown. The triangles are calculated values, the dashed lines are quadratic fittings, and the shaded regions correspond to experimental results.[8]

Besides electric fields, strain can be another degree of freedom to tune the hyperfine interaction strength. The application of strain to a Si film can be achieved through epitaxial growth on a $Si_{1-x}Ge_x$ alloy substrate along the (001) direction. Because the lattice constant of Ge ($a_{Ge} = 5.66$ Å) is larger than that of Si ($a_{Si} = 5.43$ Å), the substrate introduces biaxial tensile strains $\varepsilon_{xx} = \varepsilon_{yy}$ in the Si film. Consequently, there is a

compressive strain ε_{zz} along the growth direction. The ratio $\nu = -\varepsilon_{zz}/\varepsilon_{xx}$ is the biaxial strain Poisson's ratio, which reads $\nu = 2C_{12}/C_{11}$, where C_{11} and C_{12} are elastic constants of Si. Here we assume that the lattice constant of the $Si_{1-x}Ge_x$ alloy varies linearly with the composition x, and adopt $\nu = 0.79$ based on the C_{11} and C_{12} of Si.[32] Therefore, the strain effect can be parameterized solely by the concentration x in the $Si_{1-x}Ge_x$ substrate. Alternatively, it can also be described by the so-called valley strain χ, defined as[33]

$$\chi = \frac{\Xi_u}{3\Delta_c}\left(\frac{a_{Si}-a_{Ge}}{a_{Si}}\right)\left(1+\frac{2C_{12}}{C_{11}}\right)x, \tag{5}$$

where $\Xi_u = 8.6$ eV is the uniaxial deformation potential,[34] and $6\Delta_c$ equals the energy splitting of the A_1 and E donor states in the unstrained Si. The Ge concentration x and χ have a linear relationship, and a larger x corresponds to a more negative χ.

As discussed in Ref. [12], strain influences the hyperfine interaction strength in Si through two effects: valley repopulation and crystal deformation. Since our potential method is a first-principles approach with full atomic relaxation, the two effects are naturally included, facilitating the investigation of the impact of strain on the hyperfine interaction. In Fig. 4, the calculated relative value $A(\chi)/A(0) = |\psi(\chi;r_0)|^2/|\psi(0;r_0)|^2$ for P donors in Si with $|\chi|$ up to 45 is plotted. $A(\chi)/A(0)$ rapidly decreases from 1 to ~ 0.35 when $|\chi|$ increases from 0 to 10, and then slowly reduces to ~ 0.17 when $|\chi|$ further increases to 45. In Fig. 4, we also show the results from previous studies for comparison, including the valley-repopulation model of Wilson–Feher,[33] the Green's function[9] and tight-binding results,[12] as well as experimental values.[9] Overall, our calculations show the best match with experiments, which further demonstrates the accuracy of the potential patching method.

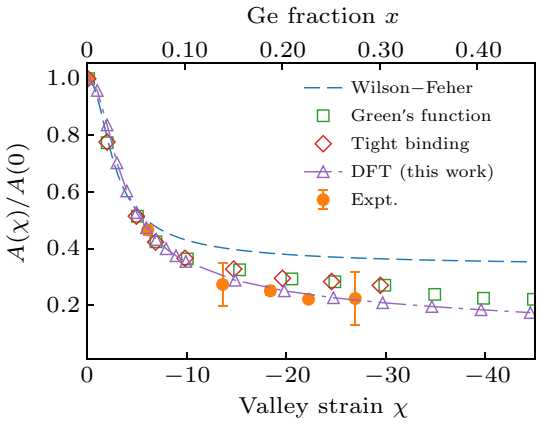


Fig. 4. The calculated $A(\chi)/A(0)$ for P donors in Si. The results from previous studies are also presented for comparison, including the valley-repopulation model of Wilson–Feher,[33] the Green's function[9] and tight-binding[12] results, as well as experimental values.[9]

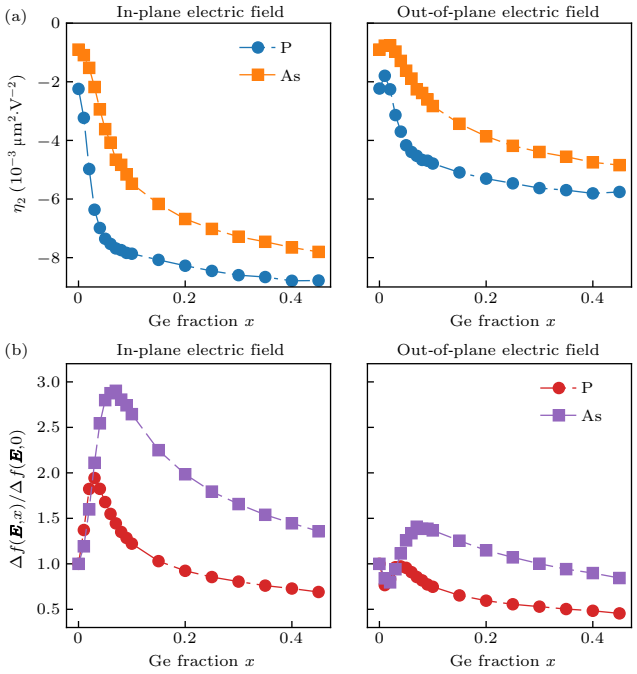


Fig. 5. (a) The Stark shift parameter η_2 of P and As as a function of x in the $Si_{1-x}Ge_x$ substrate for in-plane and out-of-plane fields. (b) $\Delta f(\boldsymbol{E},x)/\Delta f(\boldsymbol{E},0)$ as a function of x for in-plane and out-of-plane fields.

Finally we investigate the control of hyperfine interaction by the combination of strain and electric field. When grown on the $Si_{1-x}Ge_x$ substrate, the in-plane directions (100) and (010) of the Si film are no longer equivalent to the growth direction (001). Therefore, the strain dependence of the Stark shift parameter η_2 for electric fields along the in-plane direction ($\boldsymbol{E}_\parallel$) is different from the case when the field is along the growth direction ($\boldsymbol{E}_\perp$). Experimentally, these electric fields can be introduced by the top and side gates.[5,12,35] In Fig. 5(a), the η_2 of P and As as a function of x in the $Si_{1-x}Ge_x$ substrate is presented. The two donors exhibit similar trends. The magnitude of η_2 increases with increasing strain. Hence, strain expands the range of the hyperfine interaction strength that can be achieved through electric field tuning. Moreover, compared with the case of $\boldsymbol{E}_\perp$ fields, η_2 is more sensitive to strain when $\boldsymbol{E}_\parallel$ is applied. In shallow donor based qubits, a locally applied electric field induces a Stark shift and changes the spin-resonance frequency by $\Delta f(\boldsymbol{E})$, which is proportional to $\eta_2|\boldsymbol{E}|^2 A$.[1] The upper bound of spin manipulation timescale is determined by Δf^{-1}.[8,12] Therefore, a faster gate with the same fidelity can be realized with a larger Δf. According to Figs. 4 and 5(a), both A and η_2 can be modified by strain. $A(x)$ decreases with the Ge concentration x in the substrate, whereas $|\eta_2(x)|$ shows the opposite trend. It is thus interesting to explore whether the donor qubits in strained Si exhibit faster gate response. This can be quantified by the ratio $\Delta f(\boldsymbol{E},x)/\Delta f(\boldsymbol{E},0)$, which equals $\eta_2(x)A(x)/\eta_2(0)A(0)$. A ratio larger than 1 indicates that the application of strain is beneficial in terms of improved

gate response. As seen in Fig. S1 in the supporting information, $A(x)/A(0)$ has a nearly linear relationship with respect to $\eta_2(x)/\eta_2(0)$, and the slope is negative. Their product is $\Delta f(\boldsymbol{E},x)/\Delta f(\boldsymbol{E},0)$ and it thus would exhibit an approximately quadratic dependence on $\eta_2(x)/\eta_2(0)$ with a negative curvature. In general, $\eta_2(x)/\eta_2(0)$ increases with x, except for the region where x is close to 0 for the case of out-of-plane field [see Fig. 5(a)]. This suggests that $\Delta f(\boldsymbol{E},x)/\Delta f(\boldsymbol{E},0)$ also depends non-monotonically on x, first increasing and then decreasing as x increases. Figure 5(b) indeed shows such a trend, except for the initial strain interval under the out-of-plane electric fields. As seen in Fig. 5(b), for the $\boldsymbol{E}_{\parallel}$ fields, $\Delta f(\boldsymbol{E},x)/\Delta f(\boldsymbol{E},0)$ is larger than 1 when $0 < x < 0.15$ for P, and in the entire range of considered x for As. For the $\boldsymbol{E}_{\perp}$ fields, while the ratio does not exceed 1 for P, it is larger than 1 in a wide range of $0.04 < x < 0.3$ for As. Hence, the introduction of strain enables faster gate operations with in-plane fields for P, and with both in-plane and out-of-plane fields for As.

4. Conclusion

In summary, we investigated hyperfine Stark shift and its strain tunability of shallow donors P and As in Si with first-principles calculations. By employing the potential patching method, it is found that a supercell with over 10^5 atoms is necessary to well describe the donor levels and wave functions. The excellent agreements with experiments demonstrated that the potential patching method is a feasible first-principles approach with a high accuracy to study wave-function-related properties of shallow impurities such as the Stark shift parameter. The dependence of Stark shift parameter on strain introduced by substrates is systematically explored. We found that the strain expands the range of the hyperfine interaction strength that can be achieved through electric field tuning. Furthermore, it is shown that the introduction of strain enables faster qubit gate operations with in-plane fields for P, and with both in-plane and out-of-plane fields for As. The findings could provide useful information for the development of quantum computing architectures based on shallow donors in Si.

Acknowledgments

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