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First principles band structure of interacting phosphorus and boron/aluminum δ -doped layers in silicon

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E-mail: qcampbe@sandia.gov**Keywords:** electronic structure, delta layers, silicon electronics, diode

Abstract

Silicon can be heavily doped with phosphorus in a single atomic layer (a δ layer), significantly altering the electronic structure of the conduction bands within the material. Recent progress has also made it possible to further dope silicon with acceptor-based δ layers using either boron or aluminum, making it feasible to create devices with interacting δ layers with opposite polarity. Using density functional theory, we calculate the electronic structure of a phosphorus-based δ layer interacting with a boron or aluminum δ layer, varying the distances between the δ layers. At separations 1 nm and smaller, the dopant potentials overlap and largely cancel each other out, leading to an electronic structure closely mimicking intrinsic silicon. At separations greater than 1 nm, the two δ layers behave independently of one another, with an equivalent electronic structure to a p - n diode with an intrinsic layer taking the place of the depletion region. One mechanism for charge transfer between δ layers at larger distances could be tunneling, where we see a tunneling probability exceeding what would be seen for a standard silicon 1.1 eV triangular barrier, indicating that the interaction between delta layers may enhance tunneling compared to a traditional junction.

1. Introduction

Atomic precision advanced manufacturing (APAM) [1, 2] makes it possible to place dopant atoms in silicon with single-atom precision [3, 4] and concentrations beyond the solid-solubility limit [5] with small width, i.e. δ layers. This fabrication technology has been investigated for use in applications ranging from quantum computing and analog simulation to more conventional digital electronics [2, 6–12]. While APAM was originally developed for placing n -type dopants (principally phosphorus, but arsenic too [13]), recent progress has included a better understanding of surface chemistries involving acceptor-bearing precursors and even the fabrication of devices with p -type dopants [14–19]. This raises the possibility of creating bipolar electronic devices entirely in silicon using both donor and acceptor based APAM processes on the same system.

There are, however, relatively few explorations of the electronic structure of silicon subject to both n - and p -type APAM doping [20, 21]. For the creation of devices based on bipolar stacks of δ layers, it is important to understand how the electronic structure of these δ layers would interact, particularly at small separation distances. One intriguing possibility is that the induced conduction bands near the center of the Brillouin zone from the P δ -layer will have their charge compensated by the induced valence bands from the B δ -layer, moving the Fermi level into the band gap and creating a direct gap semiconductor within silicon. Conversely, the relevant defect potentials may interfere with one another, producing an electronic structure more closely resembling that of intrinsic silicon. This possibility strongly affects the understanding of tunneling in bipolar devices, where it is important to understand the conditions that enhance or suppress tunneling.

Prior theoretical work on the electronic structure of δ -layers used density functional theory (DFT) and primarily focused on calculating the band structure of individual δ layers. DFT has been used to

predict the electronic structure of phosphorus δ layers in silicon [22–25], with essential features of these predictions subsequently confirmed experimentally [26–33]. Together, these investigations showed that phosphorus δ layers introduce a metallic impurity band below the bulk conduction band edge. A similar convergence between DFT calculation and experimental characterization was also recently observed for Sb δ layers [34]. Recently, Campbell *et al* have analyzed DFT band structures for δ layers comprised of boron or aluminum [35]. They reported a similar, but inverted change in the band structure, in which an impurity band is formed above the bulk valence band edge and the Fermi level is located within these bands. The success of DFT in describing the electronic structure of δ -doped layers suggests that extending this methodology to include the interaction of donor and acceptor δ -doped layers will provide a useful first approximation of the electronic structure of multiple δ -doped layered structures.

In this manuscript, we use DFT to predict the electronic structure and local density of states (LDOSs) of interacting phosphorus and boron/aluminum δ -doped layers in silicon, building upon previous work that has only looked at a single type of δ -doped layer. We use the strongly constrained and appropriately normed (SCAN) exchange-correlation functional [36] as a reasonable compromise between the computational cost of more accurate treatments of screened exchange (e.g. hybrid functionals) and the inaccuracy of more simplistic semilocal treatments, again providing novel results. Our calculations predict that each layer creates a δ potential that hosts an impurity band, with the opposite charges compensating and mutually reducing the binding energies relative to the band edges. The extent to which the binding energies of the impurity bands are reduced is a function of the distance between the δ layers. At smaller separation distances <1 nm, the two δ -layers largely compensate each other and the electronic structure most closely resembles that of intrinsic silicon, making a direct gap unlikely. At distances >1 nm, the two layers become essentially independent. At these larger distances, the δ layers essentially form the electronic structure of a p - n junction with an intrinsic layer of silicon comprising the depletion region. We use the local potentials calculated within DFT to estimate the interlayer tunneling probability as a function of the separation between layers. It is enhanced relative to the tunneling probability for a triangular barrier with a height of the intrinsic silicon band gap (1.1 eV), indicating that interactions between the δ layers do lead to outcomes that would not be achieved with traditional diodes.

2. Methods

All of our calculations are based on 2×1 Si(100) slabs (using the cubic unit cell as our base), as seen in figure 1(a). Two δ -doped layers are placed within the silicon at $1/4$ monolayer coverage. Within these layers, all dopant atoms are placed substitutionally. The rest of the supercell is pure silicon and we do not consider other features that might be expected in fabricated devices (e.g. other impurities, including the hydrogen or chlorine atoms that might be present due to the APAM doping process). The supercell is 21.8 nm long, and we evaluate pairs of δ -doped layers separated by as much as 10 nm. The periodic boundary conditions used in our calculations introduce an infinite array of images of each δ -doped layer, with the closest being 21.8 nm away on either side of the (100) axis. Prior analysis of single layers has found this distance to suffice for converging the effects of these images [22, 35].

All electronic structure calculations are done using the QUANTUM ESPRESSO package [37]. We use the SCAN [36] approximation to the exchange-correlation functional as implemented by Yao and Kanai [38]. As shown in figure 1(b), we predict a band gap of 0.98 eV for a pure silicon supercell. This is only slightly below the experimental value [39] of ≈ 1.1 eV, suggesting that estimates of other features of the band structure might achieve a similar degree of accuracy. We use kinetic energy cutoffs of 680 eV and 2721 eV for the plane-wave basis sets used to describe the Kohn–Sham orbitals and charge density, respectively. We use a $2 \times 2 \times 1$ Monkhorst–Pack grid [40] to sample the Brillouin zone in our initial self-consistent calculation and then a $4 \times 4 \times 1$ Monkhorst–Pack grid for non self-consistent calculations before band structures are calculated. We reference all energies to the conduction band minimum (CBM) of the intrinsic silicon for any given structure. Unless otherwise noted, the atomic positions are relaxed according to Born–Oppenheimer forces and considered converged below 0.5 eV nm^{-1} . The cell size is kept fixed, mimicking the embedding of the δ -doped layer within the larger silicon structure. Band structures and LDOSs are then calculated for each structure.

The use of a supercell leads to significant folding of the Brillouin zone of the usual bulk two atom primitive cell. See the discussion by Drumm *et al* [24] for detailed interpretation of these band structures in δ -doped layers. We illustrate the Brillouin zone used for this work in figure 1(c). Because of the significant Brillouin zone folding, we only plot out to half the direction of the special points, i.e. $0.5 X = (0,0,0.5,0,0)$ in crystal reciprocal coordinates. It has previously been shown that the key characteristics of the band diagram can be captured near the Γ point when examining DFT supercells for δ layer calculations [41].

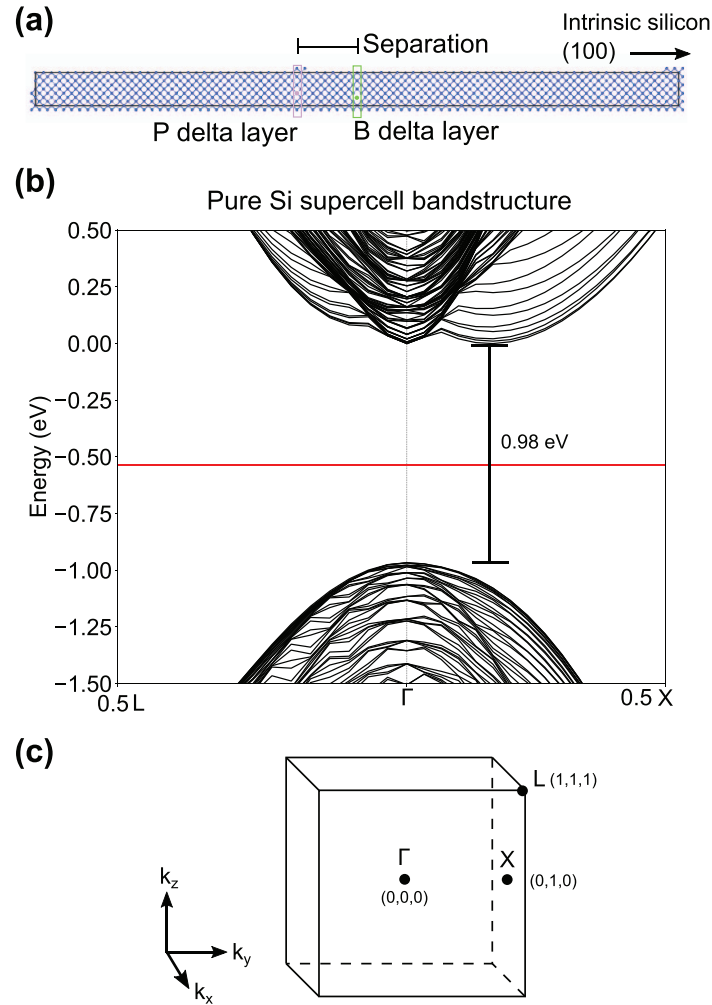


Figure 1. (a) The supercell used throughout this manuscript, indicating the P and B δ layers and the distance separating them. The horizontal axis corresponds to the (100) direction. (b) The band structure of a pure silicon supercell. Because we are using a supercell, the more familiar Brillouin zone for a two-atom primitive cell is folded in on itself. The red line represents the Fermi level of the system. (c) The Brillouin zone for the supercell, labeling high-symmetry points with crystal reciprocal coordinates. The length of the box in the k_x direction, associated with the (001) direction of the supercell is exaggerated for clarity. Given the significant length of the axis in real space, this dimension is essentially negligible in reciprocal space.

In appendix A, we show the band structures predicted for a single boron, aluminum, or phosphorus δ -doped layer using the same supercell and exchange correlation functionals employed throughout this work. These results can be used to clearly isolate the impact of a single δ -doped layer from the interaction of the multiple layers reported throughout this work. In appendix B, we show the doping potentials for boron and aluminum δ -doped layers interacting with a phosphorus δ -doped layer for each of the structures.

3. Results

3.1. Band structure and LDOS of boron–phosphorus δ -doped layers

The band structure of a pair of phosphorus and boron δ layers separated by a single atomic layer (0.124 nm) is shown in figure 2(a). At this range the layers compensate each other, leaving the material behaving largely as intrinsic silicon. The calculated distance from the top of the valence band to next band higher in energy is reduced slightly from 0.98 eV to 0.86 eV. It should be noted that the band diagram of two spatially separated δ layers can be somewhat misleading, as the z direction of the Brillouin zone is highly compressed. While the band structure appears to show a direct gap, we can see in the LDOS that the donor and acceptor δ potentials are spatially separated within the larger structure. Nonetheless, simulations of the electronic transport in similarly spatially separated bipolar devices have shown that band gap narrowing likely plays a significant role in the resulting device behavior, [21] so we still report on the energetic separation between the donor and acceptor δ bands in figures within this work. We avoid directly referring to this as a band gap since an electron would typically still need ≈ 1 eV

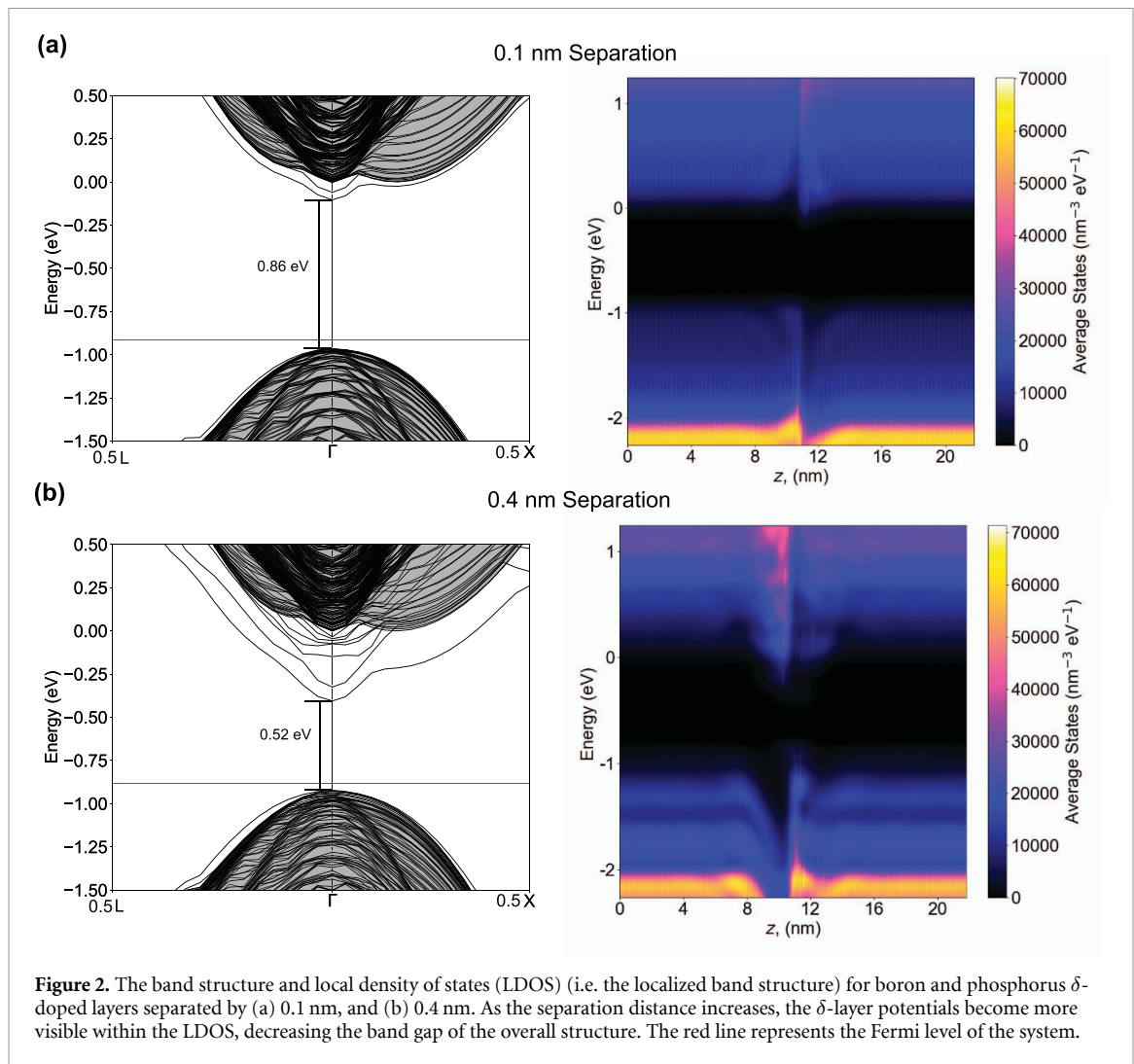
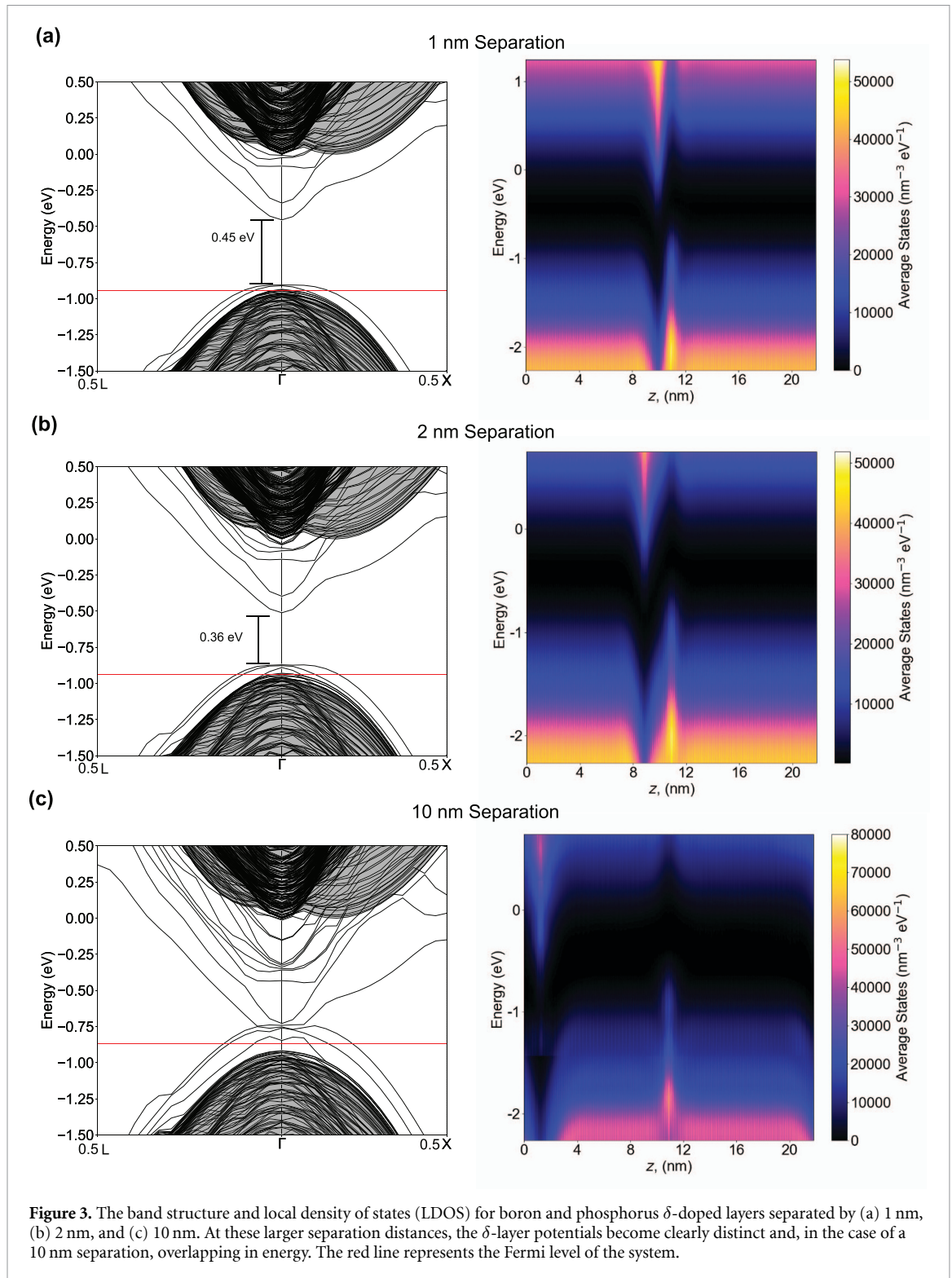


Figure 2. The band structure and local density of states (LDOS) (i.e. the localized band structure) for boron and phosphorus δ -doped layers separated by (a) 0.1 nm, and (b) 0.4 nm. As the separation distance increases, the δ -layer potentials become more visible within the LDOS, decreasing the band gap of the overall structure. The red line represents the Fermi level of the system.

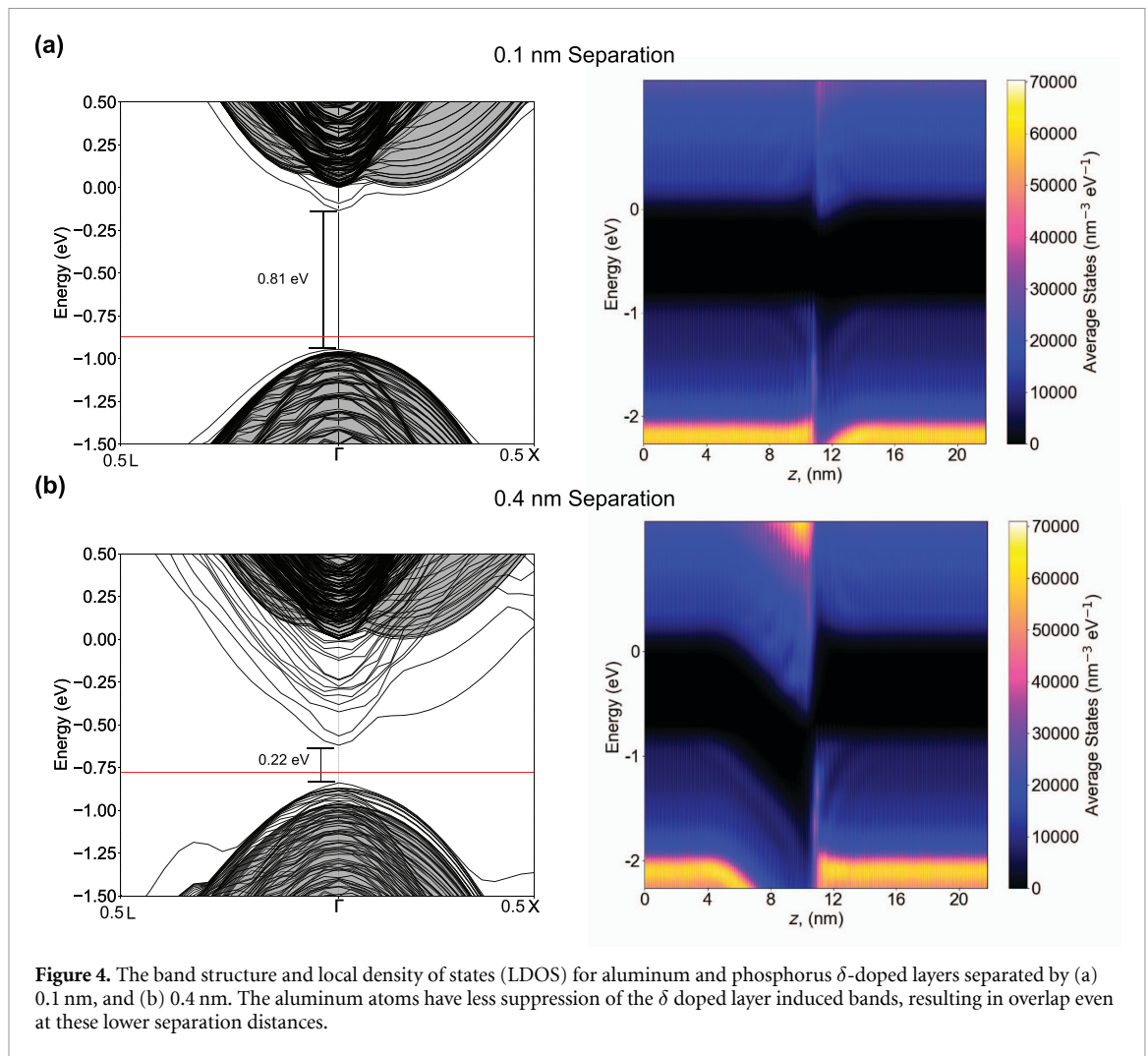
energy to move directly from the valence band to the conduction band, according to the LDOS shown in figure 2(a). Given the strong charge screening at this short separation, the δ potentials more closely resemble two adjacent triangular potentials in the corresponding LDOS diagrams. This separation distance is likely too small to be precisely achieved experimentally, but might be approximated through a sequence of dosing a silicon surface with one dopant precursor, annealing to incorporate it, and repeating the sequence with a different precursor without depositing silicon between dosing sequences.

At a separation of 0.4 nm, the δ potentials become much less suppressed, as seen in the band structure and LDOS in figure 2(b). This increase in the prominence of the δ -doped layers can be attributed to the intervening silicon layers between the donors and acceptors screening the charge from each other. The energetic distance from the boron δ layer peak to the phosphorus δ layer peak further narrows to 0.52 eV. Furthermore, the δ potentials are now clearly visible in the LDOS in figure 2(b), showing a distinct protrusion for the phosphorus δ layer in the conduction band, and a lower magnitude, but still distinct protrusion in the valence band from the boron δ layer.

At separations of 1 and 2 nm, shown in figures 3(a) and (b), respectively, the different δ layers become clearly distinct in the resulting LDOS diagrams. At 1 nm, the induced VBM from the boron δ -doped layer becomes clearly visible, shifting the Fermi level of the material within the valence bands. This is reflected in the energy difference from the boron δ layer peak to the phosphorus δ layer peak shifting to 0.45 eV at 1 nm, and clearly visible δ potentials in the LDOS in both the conduction and valence band. This trend is continued at 2 nm, with an energy difference between the boron δ layer peak to the phosphorus δ layer peak of 0.36 eV and slightly less sharp δ potentials in the LDOS. The two δ -doped layers are still interacting and suppressing the expression of each other, but this suppression reduces with separation, thus explaining the gradually decreasing energy between the boron and phosphorus δ layer peaks.



At a distance of 10 nm, however, the two δ -doped layers are fully independent. This leads to the induced valence and conduction bands from the δ -doped layers overlapping in the middle of the band gap, as shown in figure 3. This is in line with what we would expect from an independent phosphorus δ -doped layer with a magnitude ≈ 0.6 eV [22] superimposed on an independent boron δ -doped layer with a magnitude of ≈ 0.4 eV [35] away from the CBM and VBM, respectively. It should be cautioned, however, that while the overall band structure for this separation looks like a metal, examining the LDOS shows that the valence and conduction band peaks are spatially confined to the δ -layer positioning and thus unlikely to directly overlap. Thus, this structure at 10 nm layer spacing is more akin to an ultra-short p - n junction, with a level of precision in dopant placement not attainable through traditional methods such as ion implantation.

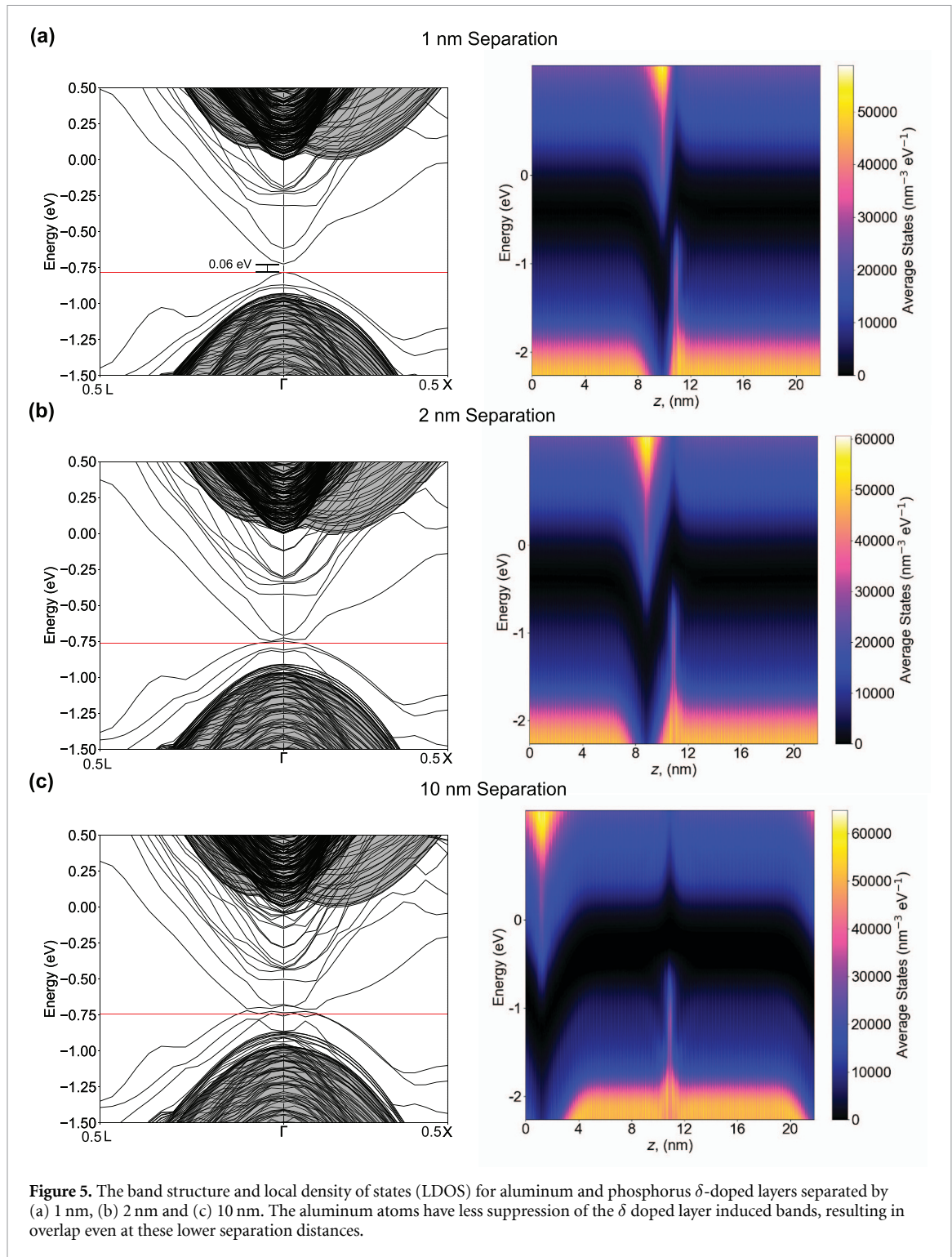


3.2. Band structure and LDOS of aluminum–phosphorus δ -doped layers

In addition to the use of boron as an acceptor for δ -doping a layer of silicon, aluminum has also been demonstrated as a potential dopant [15]. We examine how these aluminum–phosphorus structures may compare with boron–phosphorus structures in figures 4 and 5, looking at the band structure and the LDOS of the material. We see that in these systems the δ -doped layer induced bands in the band structure are less suppressed by each other than the structures doped with phosphorus and boron, leading to more strongly overlapping band structures. In appendix B, we explore the doping potentials that are generated by these boron–phosphorus and aluminum–phosphorus structures. We demonstrate that boron induces more stress in the surrounding silicon than aluminum does. This observation can be used to help explain the significantly lowered amount of suppression of the δ -layer induced bands with aluminum compared to boron, and generally cleaner valence and conduction peaks in the resulting LDOS. Stronger displacement from the boron δ -doped layers can lead to small atomic variation in the position of nearby silicon atoms, which can help screen the potential from the δ -doped layers from extending as far. Overall, however, these structures largely resemble the same behavior seen in the boron and phosphorus δ -doped layer structures, with the energy between the acceptor and donor peaks lowering as the separation increases. The LDOS for these systems also remain similar, with distinct acceptor and donor peaks forming at δ layer separation distances >1 nm. We hypothesize that an arsenic–boron system or arsenic–aluminum system (or additional combinations moving further down the periodic table) would continue the trend of lowered suppression of the δ -layer induced bands.

3.3. Carrier transport through tunneling between δ -doped layers

Given the spatially separated nature of the δ -layer peaks, if there is any charge carrier movement between the layers (absent the application of any bias on the system), one avenue is tunneling. The cost of an electron tunneling to the opposite polarity δ -doped layer is dominated by overcoming the potential barrier induced by the interacting structure. We can approximate the tunneling probability of a single



electron sitting with energy E at the phosphorus δ -doped layers moving to the boron δ -doped layer using [42]

$$T(E) \simeq \exp \left[-2 \int_{z_1}^{z_2} |k(z)| dz \right], \quad (1)$$

where z_1 and z_2 are the starting and ending point of the tunneling respectively (placed at the location of each of the δ -doped layers), and

$$k(z) = \sqrt{\frac{2m^*}{\hbar^2} (V(z) - E)}. \quad (2)$$

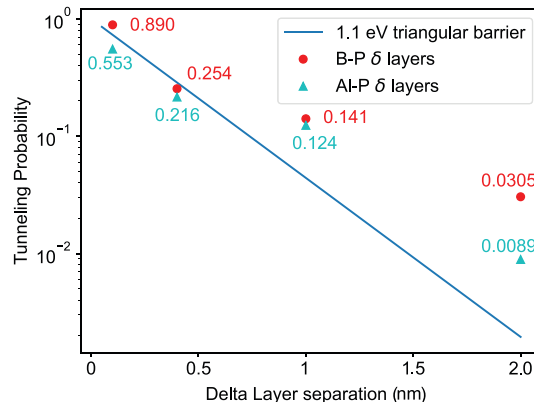


Figure 6. Calculated tunneling probability for an electron in one of the δ -layers tunneling into the other δ -layer as a function of the separation between the δ layers. The tunneling probability calculated based on the actual potential measured from the DFT calculations is higher than a pure 1.1 eV triangular barrier of the same length due to the interaction between the δ layers.

Here, m^* is the effective mass of the electron, and $V(z)$ is the potential of the system as a function of the z , position. We assume an effective mass of $m^* = 0.19m_e$, where m_e is the standard mass of an electron, matching the standard transverse mass of an electron in silicon, and the tunneling is solved for a single electron wavefunction potential landscape $V(z)$. We can conveniently abstract a $V(z)$ function from our DFT LDOS calculations (which are shown in appendix C), and numerically integrate to calculate the tunneling probability in our systems. We then compare this to the tunneling that would be expected for a pure triangular 1.1 eV barrier in figure 6.

Notably, due to the interaction between the two δ -doped layers, the tunneling probability remains higher than would be expected for a pure triangular barrier. This trend is particularly pronounced for longer separation distances. We predict the tunneling probability of a boron and phosphorus δ -doped layer separated by 1 and 2 nm is 0.141 and 0.0305, respectively. While these are not large probabilities, they are significant enough that a reasonable number of electrons may tunnel through. The tunneling rate in aluminum and phosphorus δ -doped structures are lower than for boron and phosphorus structures due to the stronger peaks induced by less relaxation of nearby silicon. This trend continues throughout the system, however, the slope of the Al-P δ layer tunneling remains above that of a 1.1 eV triangular barrier. We note that these results are before any potential bias is applied to the system, which could be used to further manipulate tunneling rates. This tunneling probability calculation is based on an electron sitting at the bottom of the phosphorus δ -layer potential well and assuming that it can tunnel to the top of the acceptor δ well. This assumption of overlapping energy levels in the donor and acceptor is clearly true at high separation distances, but seems inaccurate for separations below 1 nm. This is particularly true for boron δ layers, where the Fermi level does not sit between the valence and conduction bands, but seems to be caught within the B δ layer. We therefore show these tunneling results merely to illustrate the possibility of an electron moving between layers, and compare how easy it would be in this system compared to a generic triangular potential well. The easiest electron movement within the given system would likely still be within a δ layer, making the behavior of the material essentially metallic around the delta layer. We next examine how easy it is to move electrons around the Fermi level of the system.

The density of states (DOSs) at the Fermi level of the system gradually increases as the separation between the boron and phosphorus δ -layers increases, as shown in figure 7. At lower separations, the DOS is quite low, as the δ -layer induced bands are suppressed and the Fermi level is located within the band gap of the larger structure. As the separation between the delta layers increases, however, the δ -layer induced valence and conduction bands increase in size and the Fermi level moves from the band gap into the valence bands. This causes the DOS at the Fermi level to increase with the separation between the materials until they appear to saturate at 1 nm separation. These higher separations are thus more likely to induce weak metallic-like behavior as electrons can easily move between bands in the valence band structure. While the aluminum–phosphorus structures have systematically lower DOSs, the trends remain the same.

3.4. Considerations when comparing DFT results to experimental systems

It should be noted that the DFT simulations provided in this work are necessarily an approximation of realistic systems with both acceptor and donor δ -doped layers. Many of the errors are unfortunately

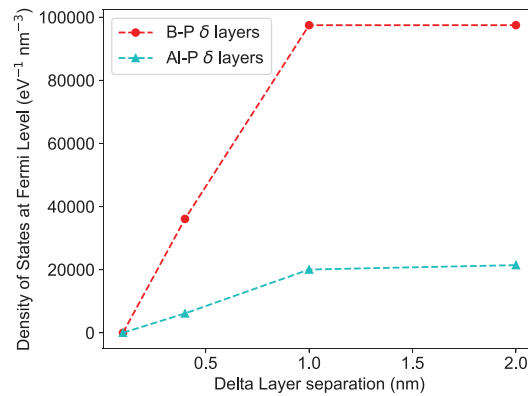


Figure 7. The density of states (DOS) at the Fermi level of the system as a function of separation between the δ layers.

inherent to any DFT-based approach for materials simulation of electronic properties. The band gap of the systems will be somewhat underestimated, an effect that has been well documented in various DFT calculations. We apply SCAN pseudopotentials [36, 38] to combat this problem, but it has not been entirely solved, as evidenced by our prediction of a pure silicon supercell of 0.98 eV. This may be particularly relevant at separation distances leading to us predicting a band structure that is continuous across the typical silicon band gap, such as the B-P 10 nm case (figure 3(c)). There may, in fact, be slight band gaps in these materials that we cannot see without significantly more computationally expensive methods. Furthermore, there is some uncertainty in the exact placement of the Fermi level, which would be dependent on the specific doping of any given sample as well as the measurement temperature. When the Fermi level is placed firmly within the typical silicon band gap (as in the 0.1 and 0.4 nm separation cases for both B-P and Al-P layers), it is particularly ill-defined within DFT and should be taken more clearly as an indication that the valence band is fully occupied and the conduction band is fully unoccupied.

There are three additional aspects of the results where the approximations necessary for DFT calculations become especially notable. The first is in the concentration effects of using a limited DFT supercell with periodic boundary conditions, which necessarily forces the concentration of dopants being modeled to be relatively high. While this high concentration is laterally correct, i.e. roughly 1/4 monolayer coverage, it is unlikely to be correct perpendicular to the δ layer. We are in fact modeling a silicon system with periodic δ layers every 21.8 nm rather than a single isolated pair of δ layers. As recently explored by Campbell *et al* [35] it can be difficult to fully disentangle the impact of δ -doped layers from the high concentration of dopants being simulated. Nonetheless, given the agreement between experimental characterization and DFT calculations of phosphorus δ -doped layers [26–31], it is reasonable to take these DFT results as good first-order approximations of the electronic structure.

The second aspect of concern is unique to the current simulation of two interacting δ -doped layers: the silicon region between the two δ -doped layers. Within our DFT simulations, we assume a pure, perfect crystalline silicon region between the two δ -doped layers. Due to the necessary low thermal budget processing to create such a structure, however, it is highly likely that this intermediate silicon region would not be perfectly crystalline, and may include a significant amount of defects. For example, silicon grown with APAM methods is known to contain oxygen and aluminum impurities [43]. This imperfect silicon structure and higher concentration of defects would likely reduce the interaction between the δ -doped layers. Further, our DFT calculations do not account for any dopant segregation that might occur during silicon epitaxy on top of the δ -doped layers.

The final aspect of concern is that while several of the systems show direct band gaps in the reported band diagrams, this represents an integration of the entire [100] direction within the system and the valence and conduction peaks are in fact spatially separated. Since the simulated slab is so large in the [100] dimension, the corresponding Brillouin zone vector is small and sampling with more than one point would not lead to clear differences in the band diagram. This band diagram should be taken to represent the electronic structure of the entire system, and not correlated with one specific region of the model in real space. To understand how the electronic structure changes in real space, we present a light absorption thought experiment using the LDOS. Based on the LDOS of these systems, a photon shined

onto the system would still have to overcome the intrinsic silicon band gap of ≈ 1 eV to be absorbed and generate a free electron and hole at any one location. Once generated, however, these charge carriers would be subject to the huge potential gradient between the δ layers and be swept to the nearest δ layer of the correct polarity. Similar analysis in InAs/GaSb superlattices, however, has shown that band gaps predicted with DFT of large supercells can match experimentally measured values, provided hybrid functionals or similar steps are taken to correct the band gap of the individual materials [44, 45]. This gives us reason to believe our methodology provides useful reference points for future experimental characterization where these δ layers could be stacked to form a superlattice analogous to the well-established III–V superlattices, manipulating defects rather than band offsets.

4. Conclusion

Motivated by recent progress in using APAM to create δ -doped layers, we used DFT to predict the electronic structure of both interacting phosphorus and boron δ -doped layers and interacting phosphorus and aluminum δ -doped layers in silicon. At separations of less than ≈ 1 nm, we demonstrate that these δ -doped layers will strongly suppress each other, leading to an effective band gap and electronic structure close to that of intrinsic silicon. As the separation between the layers increases to around 1 nm, the suppression decreases, and distinct δ potentials can be seen at the site of each layer, essentially creating a p – n diode with an intrinsic layer of silicon in the place of the depletion region. This decrease in suppression manifests as a change in the effective band gap that can be tailored by controlling the amount of silicon between the δ -doped layers, ranging from 0.36 eV for 2 nm spacing to 0.86 eV for 0.1 nm spacing. However, the CBM and VBM are spatially separated, so carrier transport between δ -doped layers likely requires tunneling or application of bias. Calculations of the δ -doped layer potentials enable us to predict the tunneling rate between the two layers, finding that the tunneling at higher separations is greater than what would be expected for a pure 1.1 eV triangular barrier. These calculations thus provide a foundation for design of silicon electronics based on interacting δ layers.

Future work in this area would need to focus on experimentally creating both acceptor and donor δ -doped layers stacked on top of each other in the same silicon device, which has not yet been demonstrated. The growth of clean, relatively defect free, intrinsic silicon between the two δ -doped layers would be a particular challenge. Further work is also needed investigating the electronic structure of δ -doped layers in other group-IV materials such as SiGe, Ge, GeSn, etc to gain a more complete understanding of the influence of varying strain and host material band structure. Validation of the band structure could be undertaken with angle resolved photoemission spectroscopy as seen in previous experimental work looking at single δ -doped layer silicon structures [26, 29, 34].

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Data availability statement

The data that support the findings of this study will be openly available following an embargo at the following URL/DOI: <https://zenodo.org/records/17186952> [46].

Appendix A. Band structures of isolated single δ -doped layers

In this appendix, we predict the band structure of a single δ -doped layer, with either boron or phosphorus dopants, using SCAN pseudopotentials for higher accuracy band gaps. We use the same supercell and calculation parameters as described in section 2 of the main text. This allows for easy comparison with our results in section 3 to determine what is an impact of interaction between the two δ -doped layers. Our results are in many ways similar to previous DFT of phosphorus δ -doped layers [22–25] and boron δ -doped layers [35], but these results are the first to use SCAN pseudopotentials [36], which provide more accurate band gaps for semiconductors.

The band structure and LDOS of a phosphorus δ -doped layer is shown in figure 8, a boron δ -doped layer band structure is shown in figure 9, and an aluminum δ -doped layer band structure is shown in figure 10. For each structure, the effects are limited entirely to the conduction band (in the case of phosphorus) or the valence band (in the case of boron). Naively, we might expect that the effects of including both a phosphorus and boron δ -doped layer would be a superposition of the phosphorus conduction band and the boron conduction bands. This description only resembles the band structures when the δ -doped layers are separated by ≥ 2.0 nm, indicating that interaction between the layers is indeed causing significant suppression of the bands at lower separations. It is notable that SCAN pseudopotentials predict that the δ potential induced by the phosphorus δ -doped layer is much more significant in magnitude than previous predictions. While the exact magnitude is likely an overestimate, it does indicate that phosphorus δ -doped layers should have an extremely large profile within our calculations. This

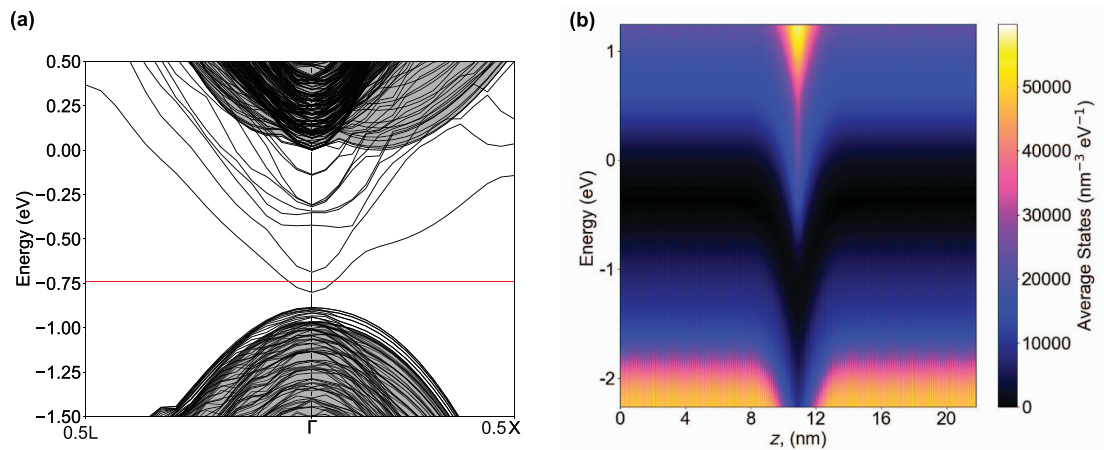


Figure 8. The (a) band structure and (b) local density of states for a single phosphorus δ -doped layer, using the same supercell and pseudopotentials as the main text.

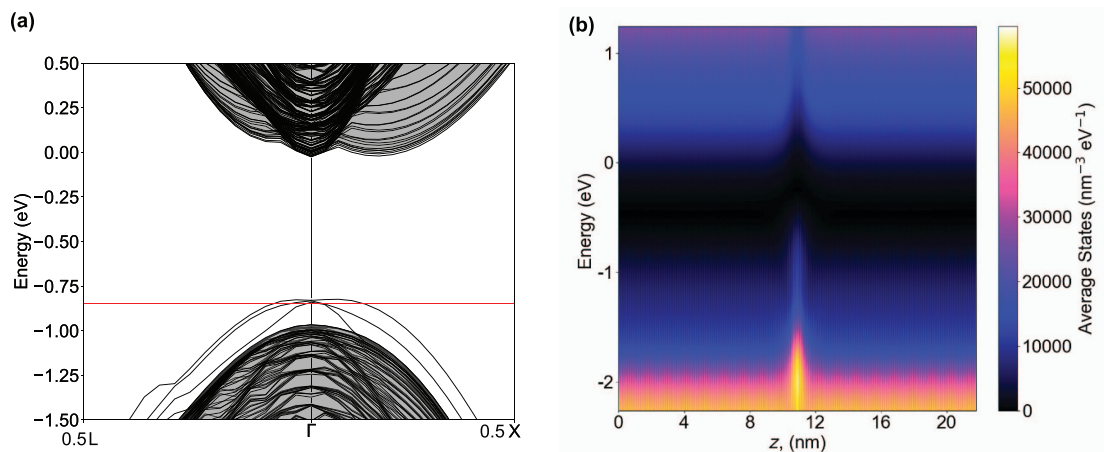
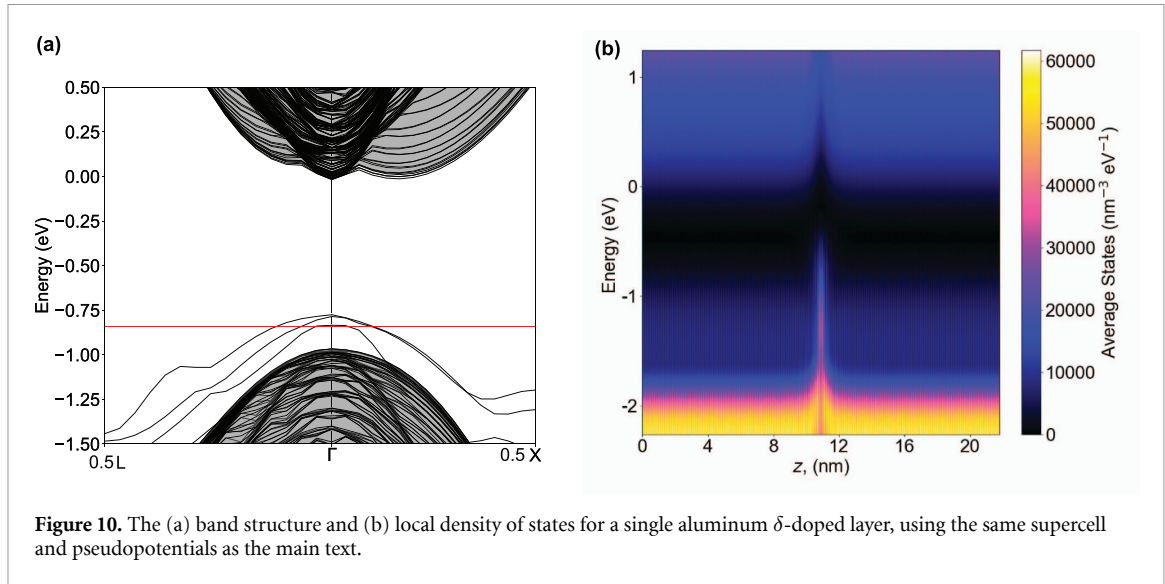


Figure 9. The (a) band structure and (b) local density of states for a single boron δ -doped layer, using the same supercell and pseudopotentials as the main text.



indicates that the suppression of the phosphorus δ -potential at low separation distances is even more significant than it may appear at first glance.

Appendix B. Doping potentials for the boron and aluminum δ -doped layers interacting with a phosphorus δ -doped layers

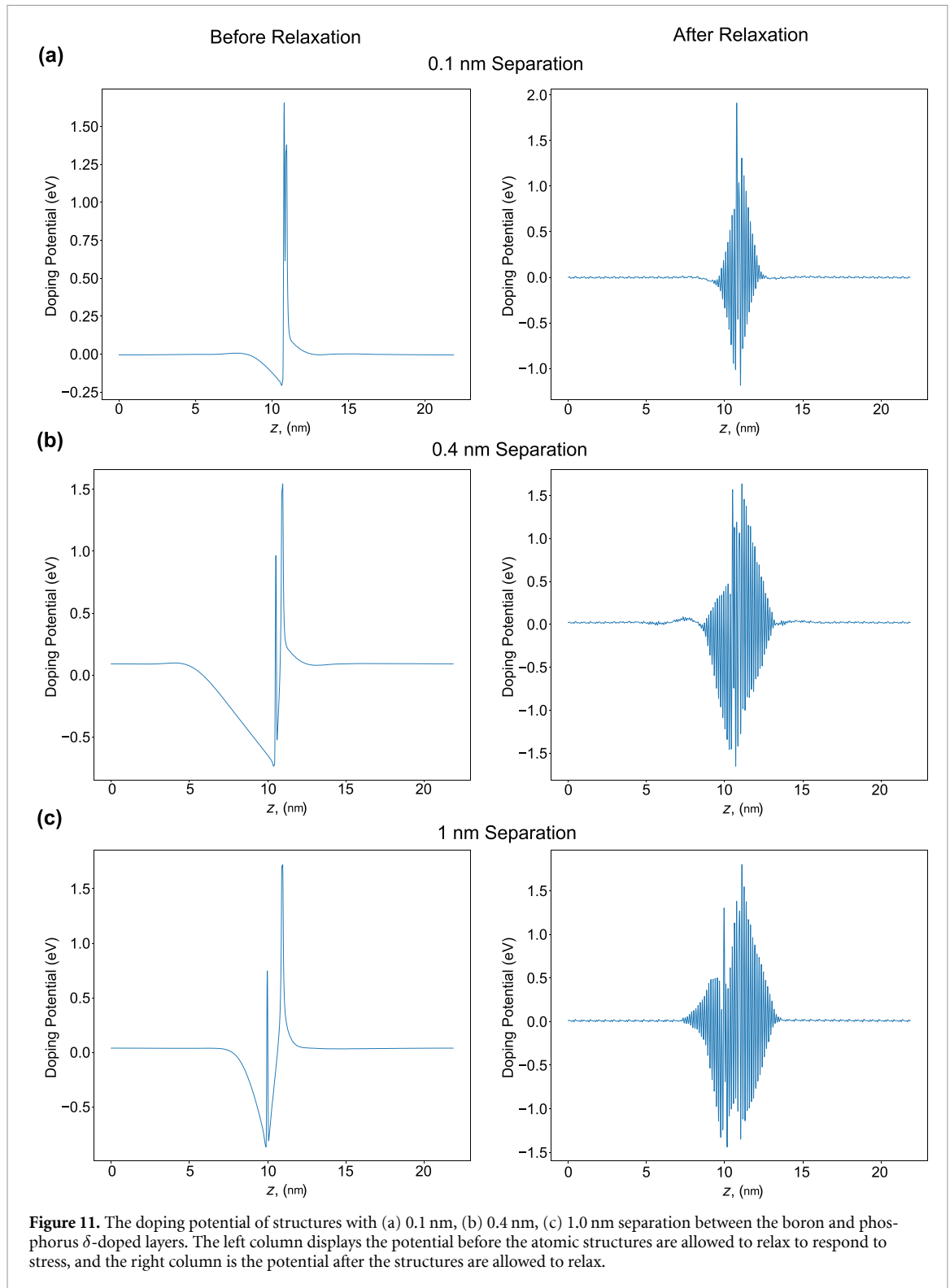
To further elucidate the nature of the δ -doped layers interaction, we plot the doping potentials for each separation distance in figures 11 and 12. These potentials are calculated by subtracting the planar averaged electrostatic potential of a pure silicon supercell from the planar averaged electrostatic potential of the system with boron and phosphorus δ -doped layers. The doping potentials calculated in the left column of each figure represent the potential before the system is allowed to relax in response to the stress that the doping atoms induce in the system. These graphs more or less follow the pattern that would be expected from the LDOS calculated in figures 2 and 3. In the right column, however, we display the potential after the system is allowed to relax in response to stress induced by the doping atoms. These potentials have a much more oscillatory character around the δ -doped layers, which is a direct result of atomic movement in response to the strain slightly altering the periodicity of the nearby silicon atoms. Similar to what is seen in [35], boron δ -doped layers feature particularly strong oscillation with the resulting δ potential being less well defined within the material compared to the phosphorus δ -doped layers. This is especially clear in the well separated structures at 2.0 and 10.0 nm separation shown in figure 12.

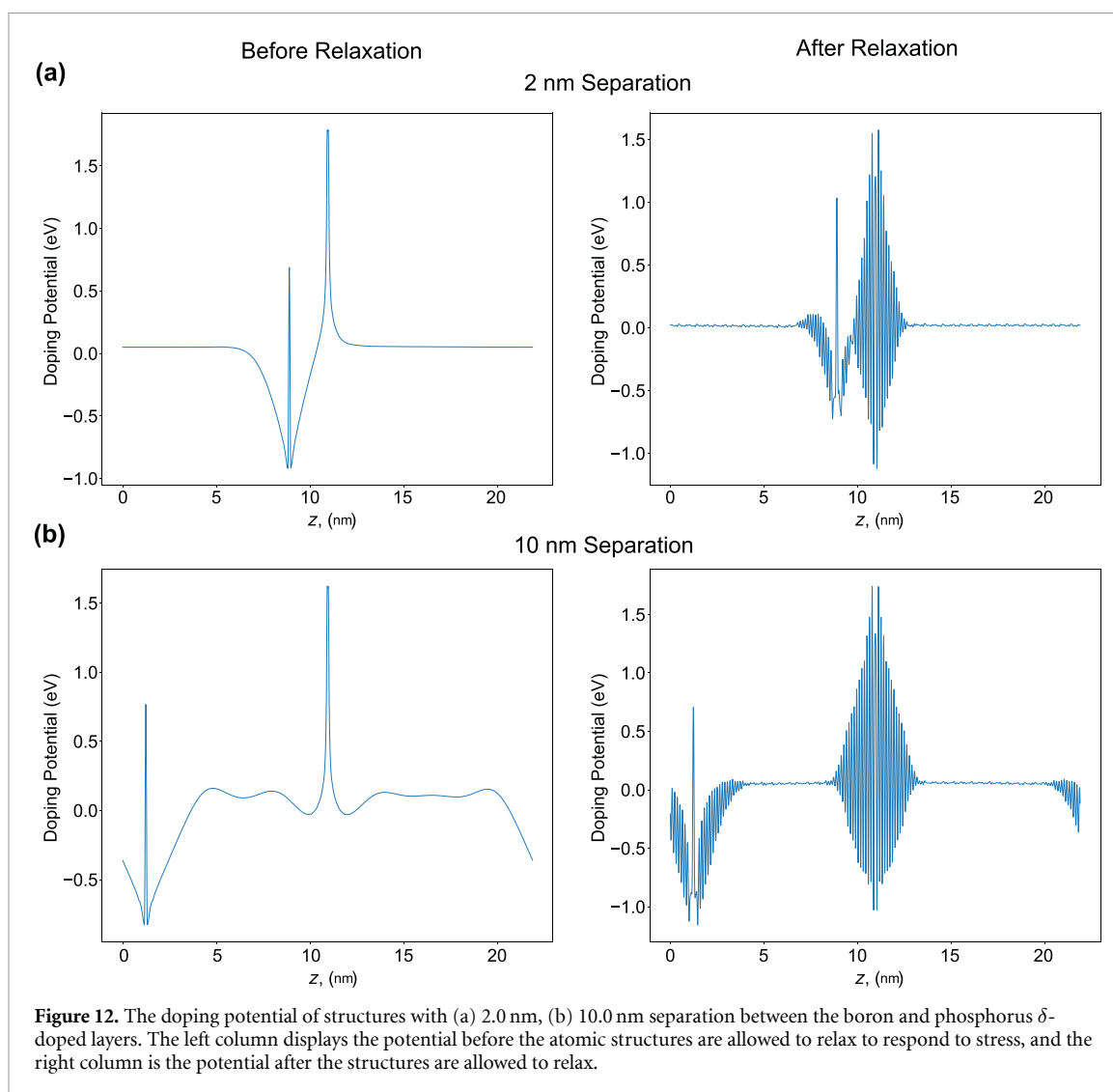
We finally examine the doping potentials of an aluminum δ -doped layer interacting with a phosphorus δ -doped layer, as shown in figures 13 and 14. The oscillatory nature of the doping potentials of the relaxed structures is much reduced, indicating much less stress is induced in response to the aluminum δ -doped layer.

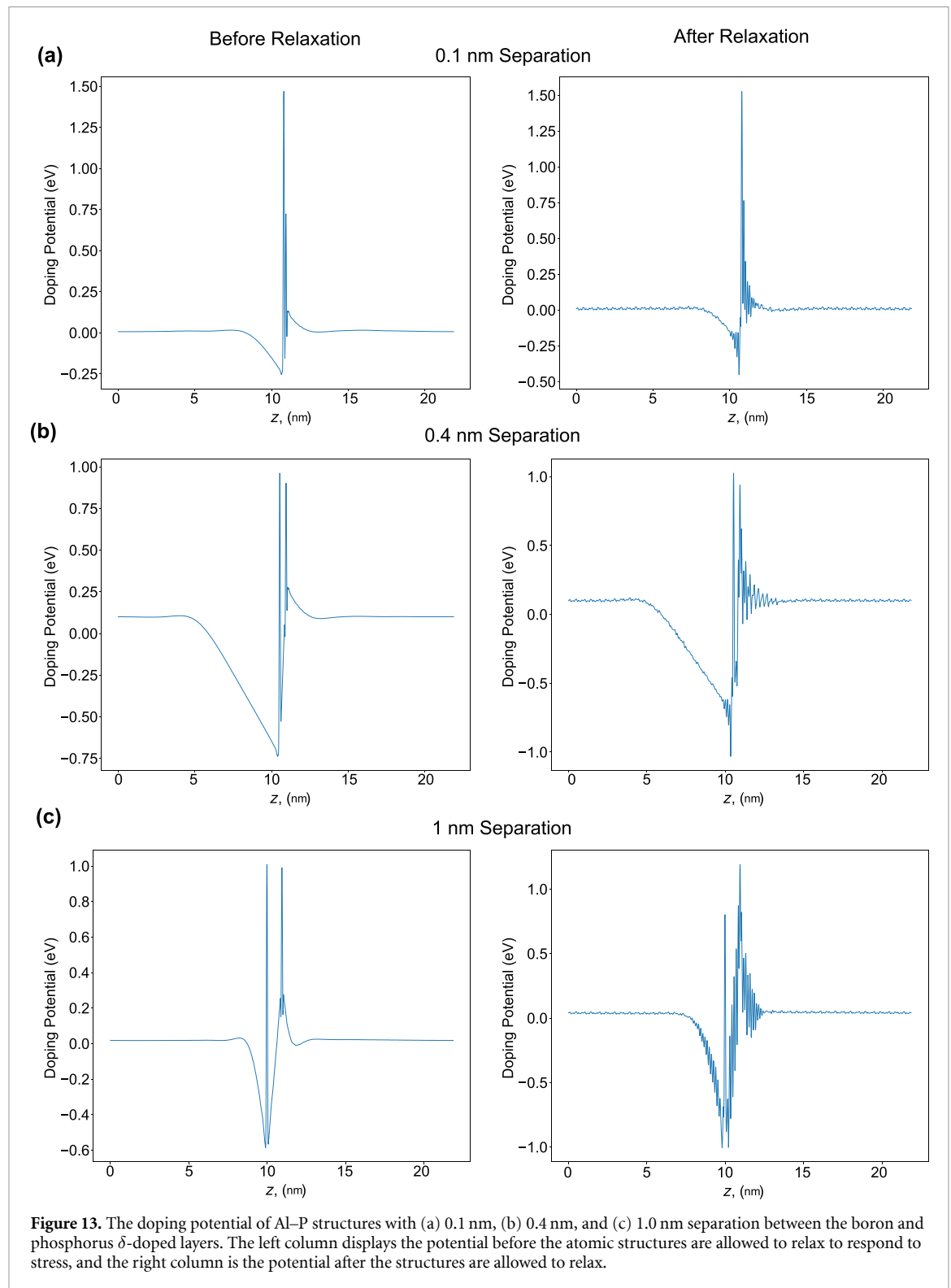
To provide a quantitative comparison between the two systems, we define a decay width σ_{doping} ,

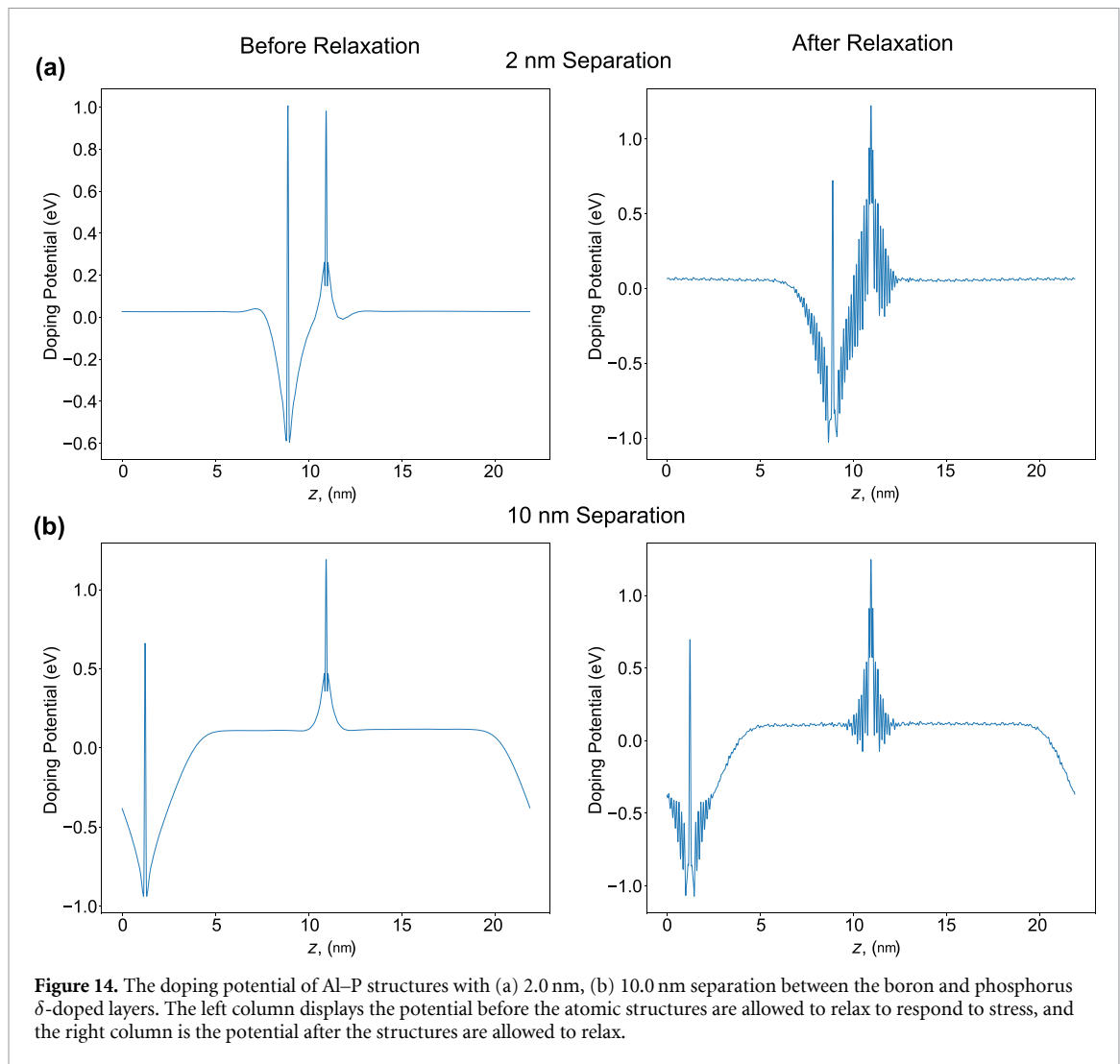
$$\sigma_{\text{doping}} = z_{\text{thr}} - z_{\text{B/Al}}, \quad (\text{B1})$$

where $z_{\text{B/Al}}$ is the z position where the B or Al δ layer is centered, and z_{thr} is the threshold z position, at which the potential oscillation is $<$ than a specified value. We choose the threshold to be a z value with potential oscillations < 0.02 V. We find that for B δ layers the average $\sigma_{\text{doping}} = 2.2$ nm, whereas for Al δ layers, the average $\sigma_{\text{doping}} = 1.6$ nm. This indicates that B δ layers induce atomic displacement in the surrounding silicon an average of 0.6 nm further away than Al layers do, which may serve as a partial explanation for why the Al–P structures tend to have more defined peaks in the LDOS than B–P structures do.



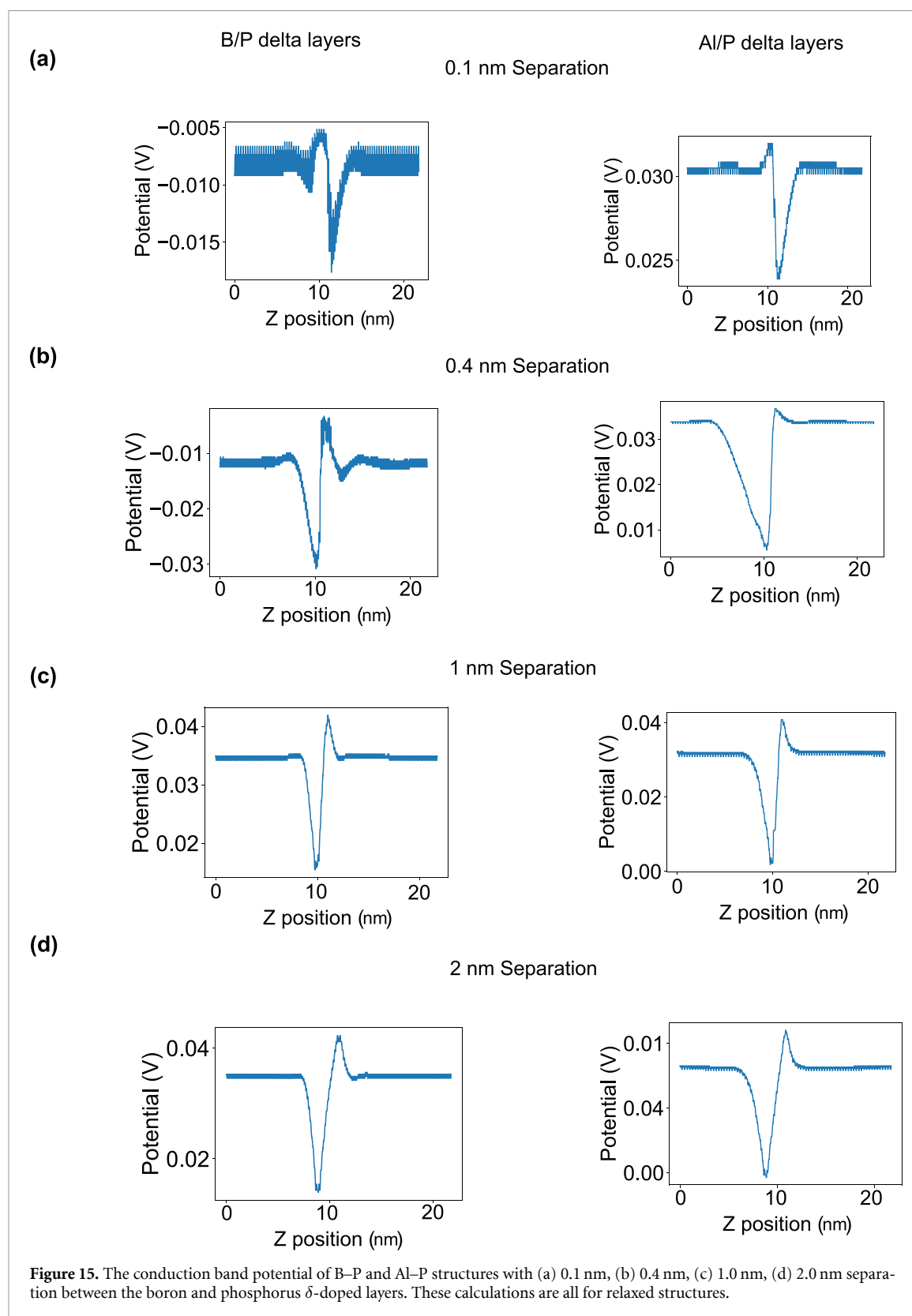






Appendix C. Tunneling potentials for the boron and aluminum δ -doped layers interacting with a phosphorus δ -doped layers

From the LDOS diagrams in figures 2–5, we can extract the outline of the conduction band minima (and corresponding valence band maxima with a potential shift) looks like. We then use this as an input potential for the tunneling calculations described in section 3.3. We show the extracted $V(z)$ plots for each system used in our tunneling calculations in figure 15.



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