Electronic Supplementary Material (ESI) for Nanoscale
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Atomistic modeling of metallic nanowires in silicon

- Supporting Information -

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1. Determination of Si buffer size to represent Si bulk

To find a size of the Si buffer that is thick enough to represent the Si bulk in simulations, we have increased the Si buffer size until the hard-wall boundaries of the simulation domain don't affect the major valleys (Γ and Δ valley) in dispersion. Fig. S1 shows the results obtained against the 0.25 monolayer (ML) doped Si:P 2D δ-layer. From Fig. S1(a) and (b), we found that, to represent Si bulk, at least 120ML thickness of Si layer needs to be considered in the simulation domain, where the energetic position of the 1Γ, 2Γ and 1Δ valley are settled within 10^{-5} meV - a convergence criterion of eigenvalue calculations in this work. Fig. S1(c) further demonstrates that, with a 120ML Si layer, the dispersion doesn't change regardless of whether a periodic boundary condition is employed along the growth ([001]) direction or not, supporting again that a 120ML Si layer is thick enough to completely protect the densely doped plane from artificial edges of the simulation domain.

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For the Si:P nanowires, 120ML Si layer is also thick enough to represent the Si bulk. To understand this, we performed simulations of a 2 Si dimer wide 0.25ML-doped [110] Si:P nanowire with two different boundary conditions, one with hard-wall boundaries along transport perpendicular directions and the other with periodic placement of the Si:P nanowire (Fig. S2(a)). As shown in Fig. S2(b), the dispersions turn out to be identical again indicating that the nanowire doesn't see the hard-wall boundaries with a 120ML Si layer.

2. Charge-potential self-consistent simulations

Electron densities in Si:P systems are expected to be large even in equilibrium at low temperatures due to the dense doping in the δ-layers. The self-consistent potential calculation, therefore, becomes the most critical factor for the accurate prediction of spatial variations of the charge density. Given the high electron density in the system, a self-consistent field calculated using the Poisson equation only is insufficient to predict the electron energy, since the mean-field theory itself fails to capture the electron exchange-correlation energy that happens due to the Pauli exclusion principle. [S1,S2] Assuming most of electrons are strongly confined near the δ-layers or highly doped channels (not within the Si layers), the Local Density Approximation (LDA), [S2] is thus used to calculate the electron exchange-correlation potential. Figure S3 shows the process of self-consistent simulations modified with the LDA correction.

The modified Schrödinger-Poisson loop used in this work has been designed to run in parallel to save simulation time with aids of supercomputers in excess of 10^5 cores (*see the TOP 500 Supercomputer Sites*, http://www.top500.org) The simulation wall-time is reduced by a two-level parallelism (Figure S4), where CPUs in the first level are used to parallelize the momentum space (*k*-space), and each core in the first level has its own CPU subgroup to spatially decompose the device domain into a 3D manner (real space). DOS and the local DOS (LDOS) are computed over the 1D (for nanowires) and the 2D (for planar doping

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devices) *k*-space with eigenvalue solvers implemented using the shift-and-invert Arnoldi algorithm, [S3] and LANCZOS algorithm. [S4] The LDOS is filled by the Fermi-Dirac function and integrated over the 1st Brillouin zone to obtain the electron density $\rho(r)$ using Eq. (1):

$$\rho(r) = \int_k \sum_n g_s \left|\psi_{n,k}(r)\right|^2 f(\varepsilon_{n,k}) dk \qquad (1)$$

where $\psi_{n,k}(r)$ and $\varepsilon_{n,k}$ are the n^{th} eigenfunction and eigenvalue at momentum k, $f(\varepsilon)$ is the Fermi-Dirac function, and g_s is the spin degeneracy. The electron charge profile is summed with the point (positive) charges of the P-ions. The total charge profile is then fed to a 3D Poisson solver built with the AZTEC linear solver package that is a free massively parallel solver library (*see* http://www.cs.sandia.gov/CRF/aztec1.html), and Finite Difference Method to discretize the simulation domain. Being subjected to the number of total electron-filling that is controlled as one of simulation input parameters, the energetic position of the Fermi-level and charge profile are determined self-consistently with the potential profile. Typical calculations require 128 cores for about 1.5 hours for the planar doping device, and 128~256 cores for 2.5~48 hours for the nanowires depending on the channel length.

References

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[S3] V. Mehrmann, and D. S. Watkins, *SIAM J. Sci. Statist. Comput.,* 2000, **22**, 1905-1925.

[S4] C. Lanczos, *J. Res. Natl. Bur. Stand.,* 1950, **45**, 255-282.

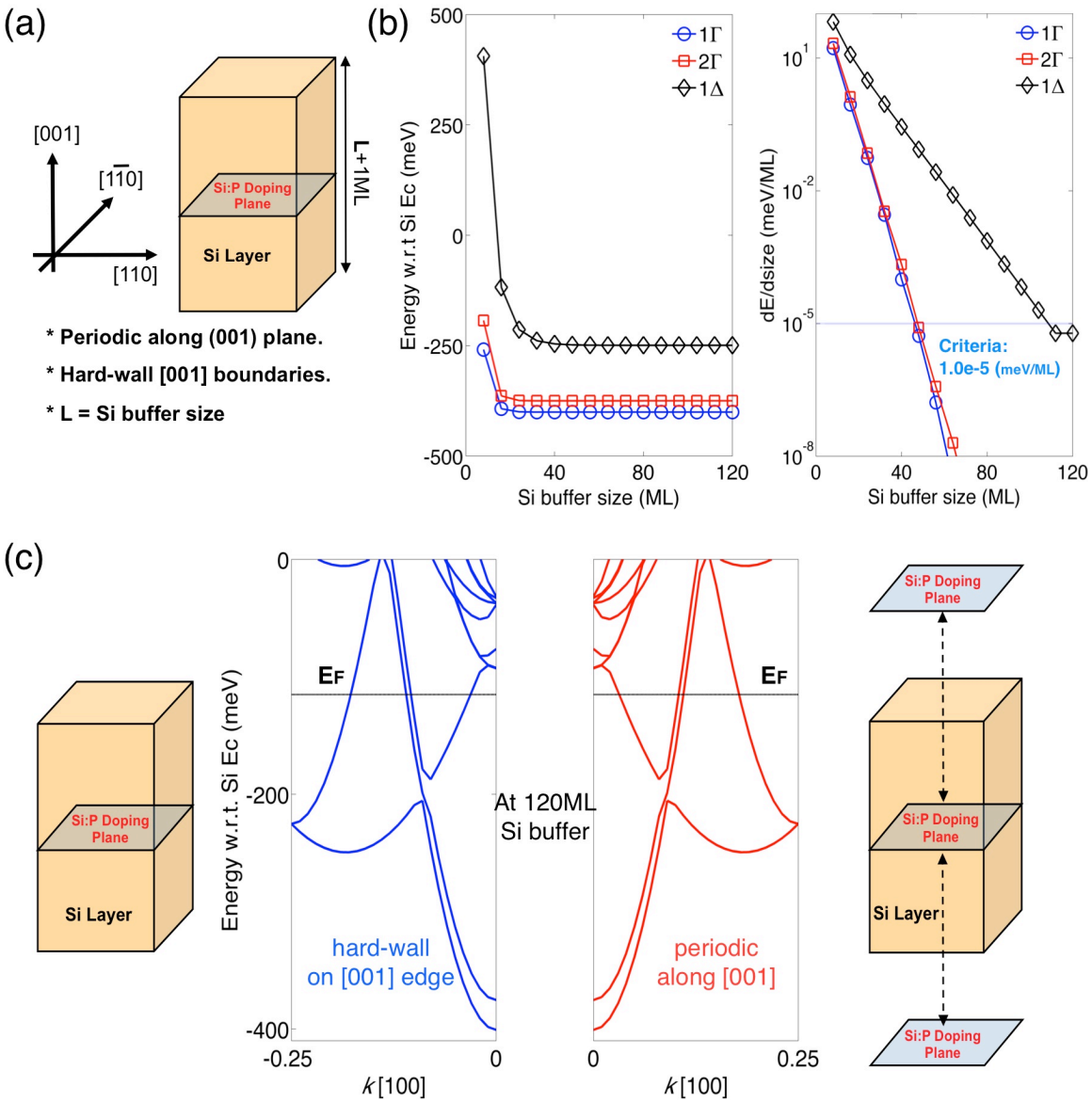

Figure S1. Determination of the Si buffer thickness needed to represent the Si bulk: (a) The thickness along the growth direction ([001]) of the Si:P δ-layers are increased until the energetic position of the major valleys are saturated. (b) The energetic position of the Γ- and Δ-valley converges within 10^{-5} meV when the Si layer is 120ML thick. (c) With 120ML thick Si layer, the dispersion even doesn't see the difference in the boundary condition. The result with hard-wall boundaries becomes identical to the one with a periodic boundary condition along the growth direction.

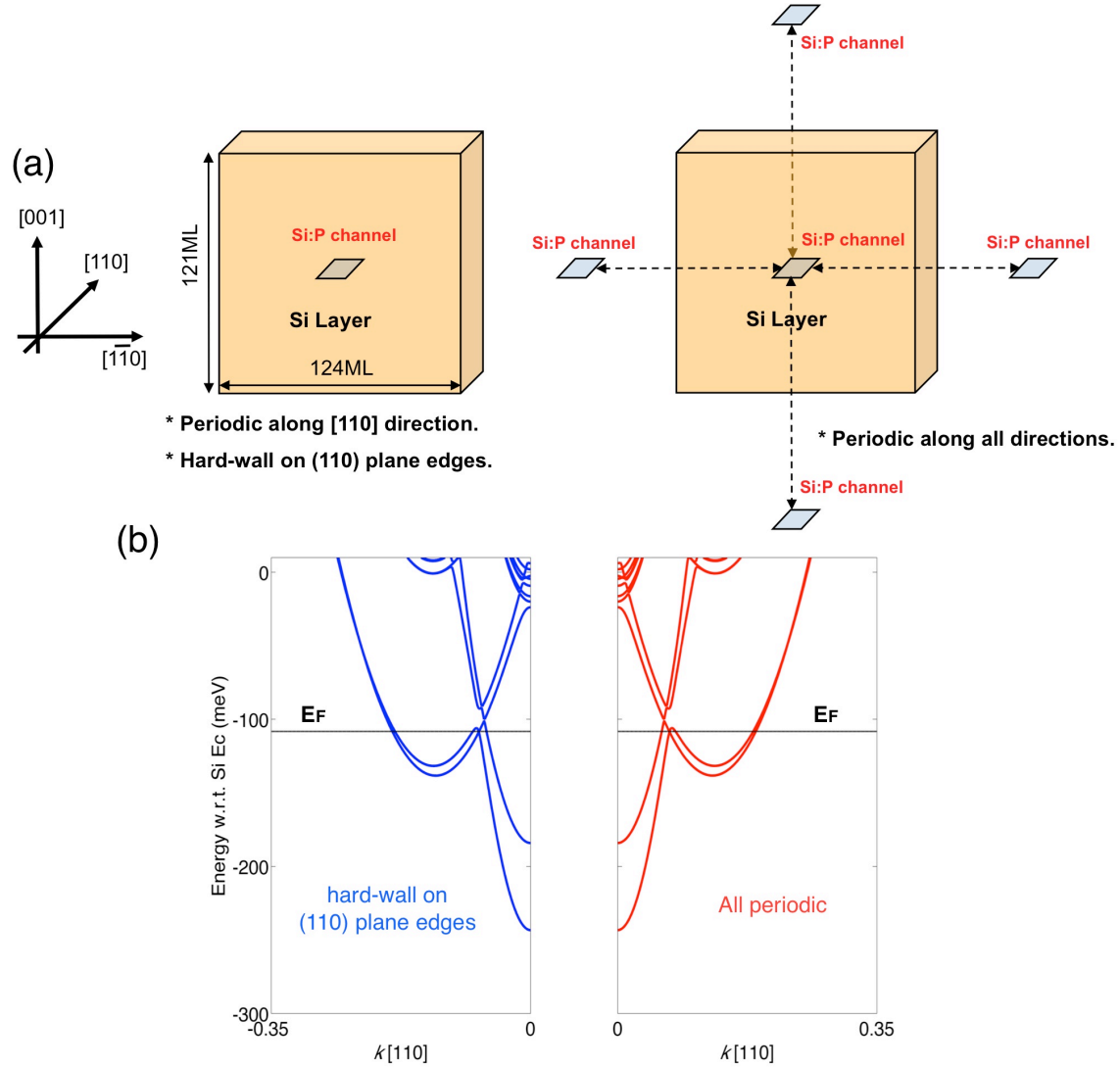

Figure S2. 0.25ML-doped, 2 Si dimer wide [110] Si:P nanowire embedded in 120ML thick Si layer: (a) Simulations are performed with two different boundary conditions, one with hard-wall boundaries and the other with a periodic placement of the Si:P channel along the transport-perpendicular directions. (b) Dispersions from two different boundary conditions are identical, which demonstrates that the densely doped channel is completely protected by 120ML thick Si layer.

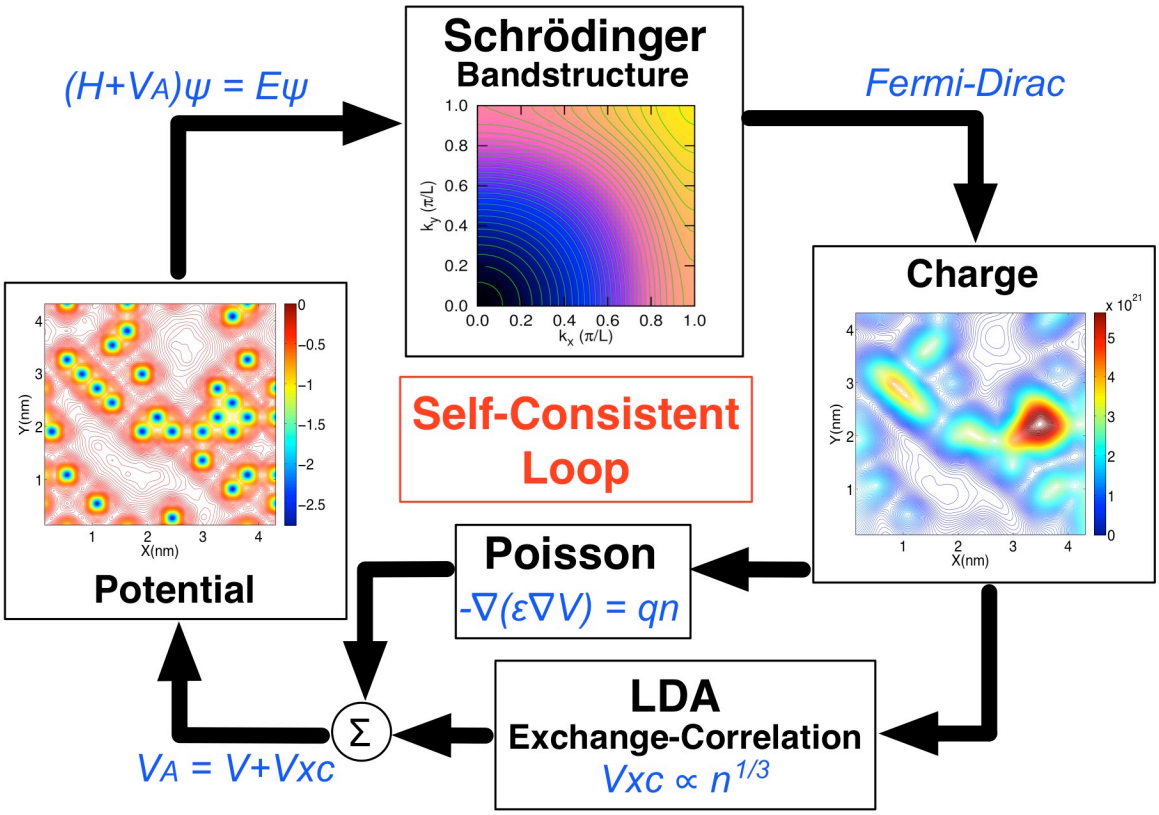

Figure S3. The process of a self-consistent calculation modified with the LDA exchange-correlation energy term. The modified process of calculations captures the electron exchange-correlation energy coming from Pauli exclusion and therefore predicts the electron energy better than just self-consistent field calculations.

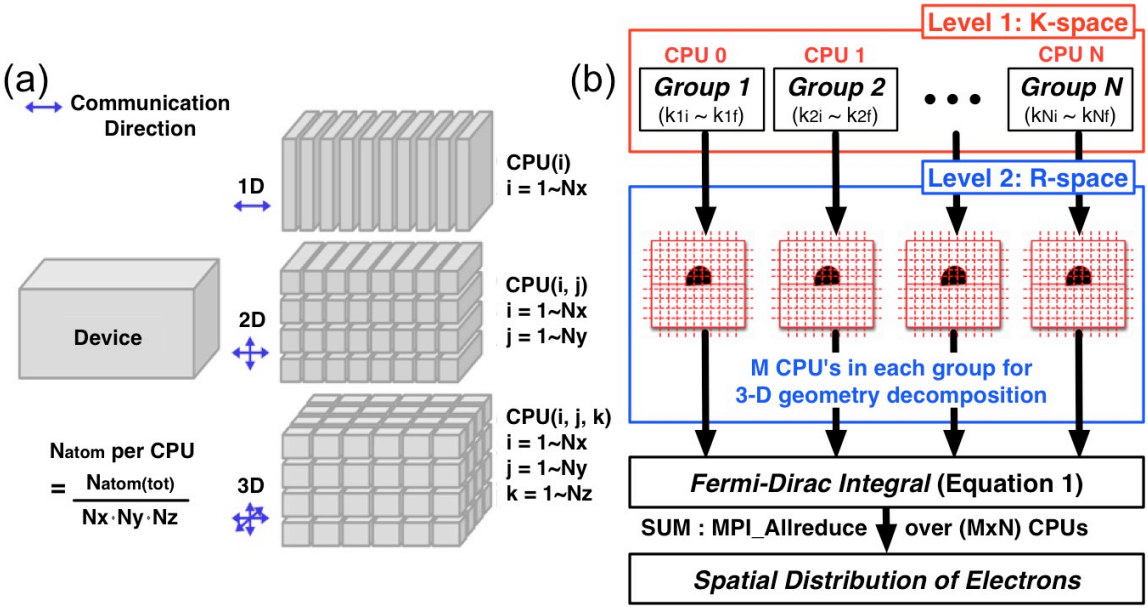

Figure S4. Illustration of the parallelism adopted to calculate the spatial distribution of electron density: (a) the device domain in a real space, is spatially decomposed into a 3D manner to increase the number of CPUs that can be utilized for parallelization. (b) a two-level parallelism where the each CPU at the 1st level parallelize the momentum space and has a sub-CPU group (the 2nd level) to parallelize the spatial domain of simulations.