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Low-current transport through dopant atom-based quantum dots in a nanoscale silicon transistor

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ABSTRACT

Quantum dot (QD) single-electron transistors, using phosphorous dopant atom QDs with radii as small as ~ 1.2 nm, are electrically characterized down to the ~ 100 fA level and over a wide temperature range, from room-temperature (RT = 300 K) to 8 K. The QDs are embedded within highly scaled ~ 5 nm silicon nanochannels. Full “Coulomb diamond,” current staircase, single-electron characteristics have been measured at 8 K, with low-current levels (~ 100 fA to 5 pA) and power (35 fW). Single-electron addition energies $E_a \sim 0.3$ eV are among the highest reported for dopant atom transistors. Unlike lithographically defined QDs, the ultra-small size of the QDs implies that both charging and quantization energies are large, each ~ 0.1 eV or greater, and the current cross-sectional area is very small, down to a 4.5 nm² dopant atom-based channel. Transitions in conduction from RT to 10 K are characterized using Arrhenius plots. Current magnitudes reduce by $\sim 10^6$, and activation energies match E_a as the device condenses into dopant atom transport channels.

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Advances in nanofabrication technology have enabled the development of quantum dot (QD) single-electron transistors (SETs) compatible with silicon large scale integrated circuits and capable of room-temperature (RT) operation.^{1–5} In the scaling limit, the device QDs can even be defined by single dopant atoms, creating a single-atom transistor within a silicon matrix.^{6–13} Dopant atom-based QDs in silicon are of great interest for the definition of ultra-low power, highly scaled nanoelectronics with one electron per bit, operating near the Landauer energy limit for energy consumption $\Delta Q = k_B T \ln 2$ per information bit.^{8,14–16} Silicon dopant atom and electrostatically induced QDs also provide highly promising systems for scalable solid-state spin qubits with long coherence time^{17–20} or higher temperature “hot qubit” operation.²¹ Silicon QD SETs may be regarded as a bridge between few-nanometer scale “classical” systems and those operating by exploiting quantum phenomena, e.g., tunneling, energy state discretization, or wave function manipulation.^{19,22,23}

RT operation in dopant atom QD SETs requires dopant energy states where the single-electron additional energy $E_a \sim 0.1$ eV or more, much larger than the thermal energy $k_B T = 26$ meV at RT, confined within deep (>0.1 eV) potential wells.²² Typically, these conditions are obtained by embedding dopant atoms in SiO₂ or Si nanoscale

channels, where the large bandgap in the former²² and increase in the donor ionization energy due to quantum confinement or nearby Si/SiO₂ interfaces in the later^{13,24,25} can create deep potential wells. The devices may then be regarded as highly scaled “single atom” versions of nanoFETs, with a nanowire or “fin” channel layout and CMOS compatibility.^{3,6} However, to ensure the presence of dopant atoms within the device channel requires high doping levels (10^{19} – 10^{20} cm^{−3}), often leading to the formation of multiple QDs within the channel and the need for gate voltage tuning for the selection of individual QDs in device operation. Furthermore, even in “classical” nanoFETs at cryogenic temperatures, the presence of any dopant or impurity atom in the silicon channel region leads to QD behavior near threshold voltage.²⁴ Any residual doping or impurity atoms in a nanoFET channel can significantly affect the “off” current, even at RT.

Both single and double QD (DQD) operation at higher temperatures (~ 200 K¹³) to RT,^{8,15} with characterization at the Landauer limit, have been demonstrated in dopant atom QD SETs. RT operation is often dominated by one or a few QDs with the smallest size and highest E_a , and the influence of QDs with small E_a is thermally overcome. However, the reduction of device temperatures can lead to rapidly increasing series resistance in the nanoscale regions leading to the QD,

turning the device “off” and preventing operation below ~ 100 K.²² While this does not affect RT nanoelectronic applications, it prevents quantum technology applications where low cryogenic temperatures are essential.

In this Letter, we demonstrate full Coulomb diamond (CD) characteristics at 8 K and the transition in conduction from RT (300 K) to 10 K in ultra-small (~ 5 nm) nanochannel dopant atom QD SETs. Results describe the behavior of few-nm scale silicon QD SETs in the ~ 100 fA/35 fW single atom, single-electron charging limit, with current flow through dopant atom induced channels. At 8 K, CDs and multiple step Coulomb staircases are measured, with very high values of $E_a \sim 0.3$ eV and very low-current magnitudes (< 100 fA to 1 pA). Data averaging is used for noise reduction. Unlike in lithographically defined QDs, single-electron charging and quantum confinement energies are comparable, due to ultra-small QD size, down to a radius of ~ 1.2 nm. Current magnitudes reduce by $\sim 10^6$ times from RT to 8 K. Arrhenius plots of device current, CD simulations, and analysis of measured data via a Morse anharmonic potential model^{26,27} allow the change in the QD radius for each charging state to be extracted. These results demonstrate the possibility of the application of large charging energy devices for low-temperature quantum technology applications.

Figure 1(a) shows a schematic diagram of a dopant atom QD SET comprising source (S), drain (D), two side gates (G), and a ~ 5 nm wide silicon (Si) fin-like nanochannel, covered by SiO_2 .⁶ The device was fabricated in a SOI wafer having heavily n -doped ($\sim 2 \times 10^{19} \text{ cm}^{-3}$ P dopant) top Si layer with an initial thickness of ~ 50 nm. Device current was determined by single-electron charging and resonant tunneling of electrons in dopant atom QDs within the channel, which was electrostatically controlled by the gates. An Al hard mask, defined in a bilayer PMMA resist using electron beam lithography,⁶ was used to form a nanochannel $20 \times 20 \text{ nm}^2$ [width (W) and length (L)] (details for extraction of these dimensions are provided in Ref. 6). This was etched into the top Si layer using a RIE SF_6/O_2 plasma. After channel etching, dry oxidation was used to form a SiO_2 surface passivation layer and reduce the Si channel dimensions to ~ 5 nm (W) $\times$ 20 nm

(L) $\times$ 36 nm height (H). A scanning electron micrograph of the completed device is shown in Fig. 1(b), where SiO_2 charging is exploited to enhance contrast and image the Si core encapsulated by SiO_2 .^{28–30}

The electrical characteristics of a dopant atom QD SET at 8 K were measured using a Keysight B1500A-B1511B parameter analyzer with a noise floor of ~ 100 fA. These are shown in a three-dimensional line plot, Fig. 1(c), and an image plot, Fig. 1(d), of the drain current (I_{ds}) vs drain voltage (V_{ds}) and gate voltage (V_{gs}). A multiple step Coulomb staircase [marked “A” in Fig. 1(c)], modulated by V_{gs} is seen in I_{ds} , e.g., at $V_{gs} = -4$ V, where three current steps at $V_{ds} = -1.2$, 0, and 1.2 V can be observed. These characteristics are attributed to single-electron transport through a dominant dopant atom-based QD within the channel. The device current is very small, with $|I_{ds}| < 5$ pA, and the device “on” resistance outside the low bias Coulomb blockade region (marked “B”) is extremely high, ~ 500 G Ω . This may be attributed not only to high tunnel resistances leading to the QD but also to an ultra-small cross section area for the current path, $A \sim 5 \text{ nm}^2$, associated with the QD size (extracted further in this Letter). Here, for a tunnel barrier of width L and $A = \pi r^2$, the tunnel resistance $R \propto (\frac{1}{A})e^{-\alpha L}$, where $\alpha = 2\sqrt{\frac{2mV_0}{\hbar^2}}$ depends on electron effective mass m and tunnel barrier height V_0 . This implies that both L and A have significant effects on R .³¹ Absolute drain current $|I_{ds}|$ vs V_{ds} and V_{gs} characteristics are shown in the color scale of Fig. 1(d), where the modulation of the Coulomb blockade forms CD regions (black regions, “1,” “2,” and “3”) associated with QD charging. Coulomb diamond edges are defined at $|I_{ds}| = 100$ fA, as lower magnitudes approach the measurement set-up noise floor. The device DC “off” power is extremely small, $\sim 100 \text{ fA} \times 0.35 \text{ V} = 35 \text{ fW}$. As the data in Figs. 1(c) and 1(d) are relatively close to the measurement noise floor, a 11-point moving average of the data was used to remove single point noise (see supplementary material S1 for the discussion of the raw data and the averaging process, and determination of CD edges).

The temperature (T) dependence of the two-terminal I_{ds} vs V_{ds} characteristics of the device from 300 to 10 K is shown in Fig. 2. This

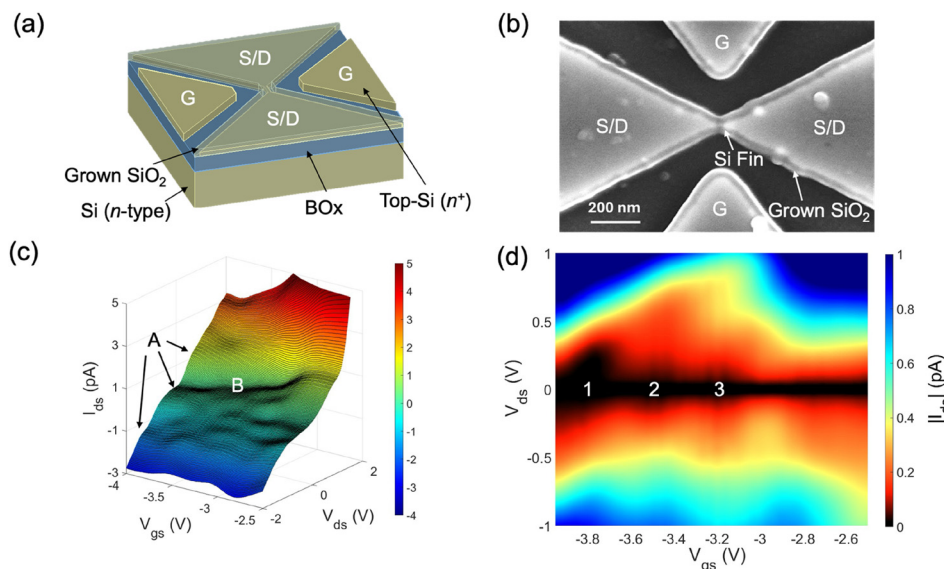


FIG. 1. (a) A schematic diagram and (b) scanning electron micrograph for a dopant atom QD SET fabricated in an SOI wafer. The device includes two gates (G), source (S), drain (D), and a channel in top Si layer (beige layer) and surrounding grown SiO_2 (transparent layer). (b) The Si nanochannel, with ~ 6 nm in width (brighter region), encapsulated by SiO_2 (relatively transparent region). (c) A three-dimensional line plot showing I_{ds} vs V_{ds} and V_{gs} characteristics for the device at cryogenic temperature (8 K) showing Coulomb staircase and Coulomb blockade characteristics, labeled as “A” and “B,” respectively. (d) Image plot with color scale showing $|I_{ds}|$ vs V_{ds} and V_{gs} characteristics where three prominent Coulomb diamond regions marked “1,” “2,” and “3.”

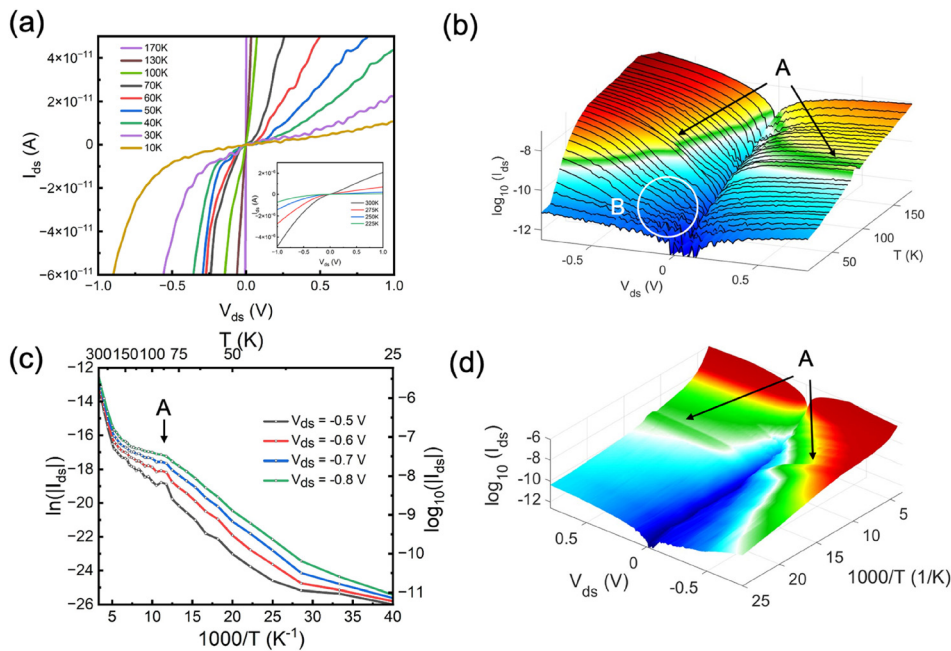


FIG. 2. (a) and (b) Two-terminal I_{ds} vs V_{ds} characteristics of the device with floating gate showing temperature dependence from 300 to 10 K. (a) The inset shows I_{ds} vs V_{ds} characteristics at cryogenic and higher temperature (225–300 K), respectively. While Coulomb staircase features are faint above ~ 200 K due to higher thermal current, the features become more pronounced below 70 K in (a) and can also be observed in (b) (labeled as “B”). (c) and (d) Arrhenius plots of $\ln(|I_{ds}|)$ vs $1000/T$ corresponding to the measurements in (a). A current peak [labeled as “A” in (b)–(d)] can be observed at ~ 85 K likely due to the electron maximum mobility in Si.

shows plots of (a) I_{ds} vs V_{ds} at nine selected values of T and (b) $\log |I_{ds}|$ vs (V_{ds}, T) . Arrhenius plots, $\ln |I_{ds}|$ vs $1000/T$, at selected values of V_{ds} are shown in (c). Finally, Fig. 2(d) shows a detailed Arrhenius plot of $\log |I_{ds}| - V_{ds}$ vs $1000/T$. $|I_{ds}|$ reduces from $\sim 1 \mu\text{A}$ at RT to $\sim 1 \text{ pA}$ or less at 10 K, a reduction of $\sim 10^6$ times. This very large change in current magnitude occurs simultaneously with changes in activation energy. Coulomb staircase features become faint above ~ 200 K due to increasing thermal current, although a high-resistance non-linear region at low bias persists up to RT. At $T < 70$ K, the Coulomb staircase [as characterized in Fig. 1(c)] becomes more pronounced [marked “B” in Fig. 2(b)]. The Arrhenius plot in Fig. 2(c) can be used to extract the maximum activation energy, associated with the highest energy barrier E_B along the conduction path. $E_B \sim 0.18$ eV between 300 and 200 K.^{32–36} A small current peak marked “A” can also be observed at ~ 85 K in (b)–(d). This peak may be associated with the electron mobility maximum in Si, due to the transition from acoustic scattering to impurity scattering near this temperature.^{37,38}

The CD dimensions in Fig. 1(d) may be used to extract values for E_a for this device. The reduction in the width/height ratio of CDs 1–3 implies a reduction in $E_a = E_c + \Delta E_k$, where E_c is the Coulomb charging energy and ΔE_k is the energy state separation due to quantum confinement or additional spin related effects.^{39,40} The CD height in the vertical axis (ΔV_{ds} , measured from $V_{ds} = 0$ V, in eV) corresponds to $\Delta V_{ds} = E_a$. Ignoring spin and using a spherical QD approximation of radius r and QD capacitance $C_\Sigma = 4\pi\epsilon_r\epsilon_0 r$, corresponding to the self-capacitance of a sphere embedded in depleted Si (relative permittivity $\epsilon_r = 11.7$), gives $E_c = \frac{e^2}{C_\Sigma} = \frac{e^2}{4\pi\epsilon_r\epsilon_0 r}$ and $E_k = z_{n,l}^2 \frac{\hbar^2}{2mr^2}$, where $z_{n,l}$ are the roots of spherical Bessel functions and m is the effective mass.^{22,39} For CD 1, $\Delta V_{ds1} \sim 0.35$ V gives $r_1 \sim 1.2$ nm, $E_{c1} \sim 0.1$ eV, $\Delta E_{k1} \sim 0.25$ eV, and $E_{a1} \sim 0.35$ eV by solving the quadratic equation for E_a vs r . Extending this approach to CD2 and 3 allows us to understand qualitatively the behavior of the QD potential well with increasing energy.

Extracted effective radii, charging, quantum confinement, and addition energies for CD 2 are $r_2 \sim 1.9$ nm, $E_{c2} \sim 0.066$ eV, $\Delta E_{k2} \sim 0.134$ eV, and $E_{a2} = 0.2$ eV, and for CD 3 $r_3 \sim 2.1$ nm, $E_{c3} \sim 0.058$ eV, $\Delta E_{k3} \sim 0.12$ eV, and $E_{a3} = 0.18$ eV, respectively. E_c and ΔE_k are of similar magnitude due to the ultra-small QD size. $E_a = E_c + \Delta E_k \gg k_B T = 26$ meV at RT, supporting RT operation in these types of devices.^{39,41,42} These values of $E_a \sim 0.18$ – 0.35 eV are larger or comparable to recent reported values for both Si QDs and other QD systems, e.g., graphene, InAs/InAsP, and nanoclusters (Table S1, supplementary material). Furthermore, the very small ~ 2 nm magnitude for effective radii and its similarity to the average dopant atom separation ~ 3 nm in our channel support the argument that the QD is associated with the P donors. The increasing value from r_1 to r_3 implies an increase in the spatial extent of the energy states, i.e., a wider effective potential well. The potential energy may be modeled using an anharmonic Morse energy potential $V(r) = D_e(1 - \exp(-a(r - r_0)))^2$, where r_0 is the location of the potential well minimum, and the energy parameter D_e and the inverse length a determine the depth and width of the potential, respectively.^{22,26} The Morse potential provides a simple physical method for QD modeling, with analytical expressions for energy states, $E_k = \hbar\omega(n + \frac{1}{2}) - \frac{(\hbar\omega)^2}{4D_e}(n + \frac{1}{2})^2$, very tractable in fitting to our E_k values. Fitting gives $D_e = 1.067$ eV and $a = 1 \text{ nm}^{-1}$ [Fig. 3(a)]. A QD potential well depth ~ 1 eV and energy state wavefunction length scale ~ 1.8 (lowest energy state)– 2.5 nm (highest energy state) are observed. These correspond to excited states within the potential, and lower energy states are not observed. Furthermore, if a chain of dopant atoms forms the conduction path, the lowered potential at $r - r_0 > 0$ and higher potential at $r - r_0 < 0$ allow the effect of “saddle” potentials between neighboring dopants, and a likely harder potential at the chain ends to be incorporated.

The experimental data in Fig. 1 are now investigated further using a plot of device conductance g_{ds} vs V_{ds} , V_{gs} [Fig. 3(b)], and data fitting

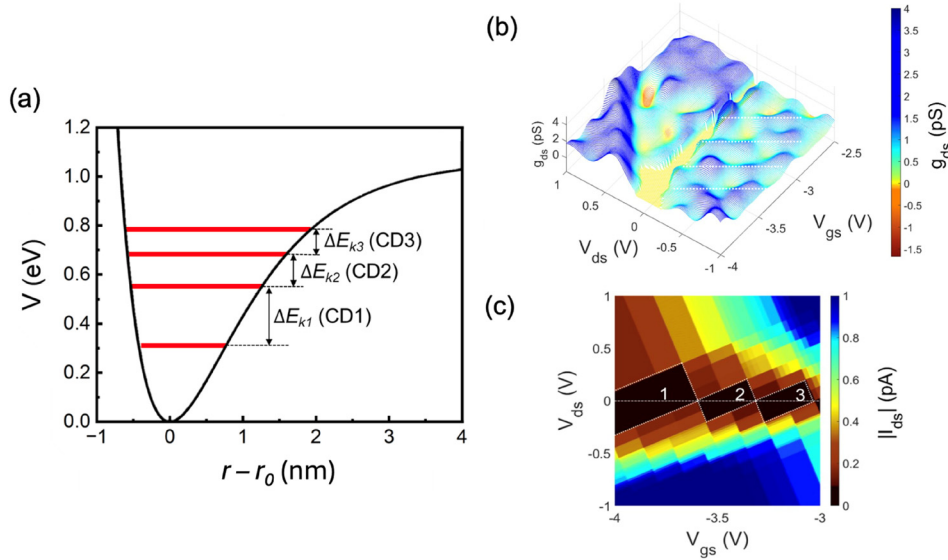


FIG. 3. (a) The potential energy $V(r)$ of the device modeled with an anharmonic Morse energy potential model. The inset equation shows the fitting of $V(r)$ where the well depth energy $D_e = 1.066$ eV and the constant parameter $a = 1.011$. (b) Conductance g_{ds} vs V_{ds} and V_{gs} characteristics for a SET-FET at cryogenic temperature (8 K) corresponding to the drain current characteristics in Fig. 1(d). In the conductance characteristics, the peaks arrange along the lines (marked by white dashed lines) of the edge of Coulomb diamond region. (c) Simulation of the electrical characteristics with similar CDs 1–3 observed in Fig. 1(d) by using extracted E_c and ΔE_k . The tunnel and gate capacitance values used in simulation were 0.25 and 1.11 aF, respectively, and the tunnel resistance value was 3 G Ω .

via single-electron CD simulation based on the master equation method^{2,43,44} [Fig. 3(c)]. Figure 3(b) shows conductance peaks along the edges of the CDs (yellow region) and at the current steps seen in Figs. 1(c) and 1(d). The Coulomb diamonds in Fig. 3(b) correspond to CDs defined within the $|I_{ds}| < 100$ fA contours (black regions) in Fig. 1(d). Conductance peaks are arranged in lines (marked with dashes) along the edges of stability regions. However, the data are complex, due to the existence of additional conductance peaks that do not show in the I - V plots of Fig. 1. Hence, the conductance plot provides evidence of the presence of multiple dopant atoms in the device channel, which influence electron transport to varying degrees. Finally, our extracted values for E_c and ΔE_k (see above) may be used for the simulation of the QD characteristics [Fig. 3(c)]. The simulation results reproduce CDs 1–3 associated with our dominant dopant atom-based QD. The presence of multiple states leads to additional diamond-like charge stability regions outside the Coulomb blockade and leads to more complex electrical characteristics, similar qualitatively to the behavior in our conductance plot [Fig. 3(b)].

The observed significant reduction of the device current with temperature and the large resistance (~ 500 G Ω) of the device may be attributed partly to the nature of quantum transport wave propagation through a narrowing junction.^{45,46} In a nanoscale constriction, only modes where the corresponding wavefunction peak fits within the constriction contribute to current through the device, and electrons in other modes are reflected.⁴⁶ When the temperature is reduced, less modes are becoming available, which contributes to increased resistance and reduction of current through the device. Finally, the activation energy, $E_B = 0.18$ eV, extracted from Arrhenius plots (Fig. 2) is of similar order to $E_a \sim 0.18$ – 0.35 eV extracted from the CDs. This is consistent with the thermal activation of electrons over the Coulomb gap in our QDs at higher temperatures > 200 K.

The high E_a value dopant atom-based QDs within our device may be associated with (i) P dopant induced states in SiO₂ regions in the nanochannel region, or (ii) isolated P donor, hydrogenic-atom like states with enhanced ionization energy in the few-nanometer wide Si nanochannel region. Such an enhancement can be due to quantum

confinement^{13,25} in the nanochannel or due to the nearby Si/SiO₂ interface.²⁴ In comparison with (ii), dopant states due in SiO₂ are less well understood. Here, density function theory calculations⁴⁷ suggest that if P–Si bonding occurs, energy states ~ 0.9 eV below the top of the ~ 9.7 eV energy gap of SiO₂ are formed. P–O bonding forms mid-gap states close to the Fermi energy, ~ 3.7 eV above the bottom of the SiO₂ bandgap. Furthermore, at our high doping concentration ($\sim 3 \times 10^{19}$ cm⁻³), mid-gap states can form due to interstitial P_x configurations.⁴⁸ These various states all form deep levels where large E_a values can occur. There is also the possibility that P–Si pairs existing in the pre-oxidation doped Si nanochannel are not substituted by P–O pairs following oxidation. This can result in QDs associated with a PSi₄ atomic configuration, surrounded by SiO₂, a situation between the cases considered in Refs. 25 and 47. Incomplete oxidation can also leave small Si nanocrystal QD in the channel, though QDs triggered by our heavy doping concentration appear more likely. Finally, multiple dopant atoms can form multiple QDs in our device. If these are at different channel locations, hence different gate coupling, Coulomb diamonds would manifest at different gate voltages. Tuning of the gate voltage can identify bias windows where a single QD dominates.

In summary, low current (~ 100 fA to 5 pA), high E_a (~ 0.35 to 0.18 eV) single-electron characteristics and energy potentials in an ultra-small (~ 5 nm) nanochannel dopant atom QD SET in silicon were investigated. Current magnitudes were very low due to transport through dopant atom states. Coulomb diamond characteristics at 8 K were measured and simulated, and the conductance transition from 300 to 10 K is characterized using Arrhenius plots. Activation energy barriers corresponded to QD electron addition energies. A Morse anharmonic potential model allowed changes in QD effective size to be characterized. The devices raise the possibility of high E_a QD devices in low-temperature quantum circuit applications.

See the [supplementary material](#) for Fig. S1 and associated discussion describing the averaging process for the raw data and the determination of Coulomb diamond edges. Recent reported values of activation

energy E_a for SETs with different island systems, are provided in Table S1.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Kai-Lin Chu: Conceptualization (equal); Data curation (equal); Formal analysis (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Writing – original draft (equal); Writing – review & editing (equal). **Wenkun He:** Conceptualization (equal); Data curation (equal); Formal analysis (equal); Investigation (equal); Methodology (equal). **Jun Hwan Kim:** Formal analysis (equal); Investigation (equal); Software (equal). **Jingbo Chen:** Data curation (equal); Investigation (equal); Methodology (equal). **Aleksey Andreev:** Conceptualization (equal); Formal analysis (equal); Funding acquisition (equal); Software (equal); Validation (equal); Writing – review & editing (equal). **Mervyn Jones:** Conceptualization (equal); Formal analysis (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Supervision (equal); Writing – review & editing (equal). **Zahid Durrani:** Conceptualization (equal); Formal analysis (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Supervision (equal); Writing – original draft (equal); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available within the article and its [supplementary material](#).

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