

# Long-range hopping in the confined electronic states of atomically constructed Cs chains on InSb(110)

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Solid-state quantum simulation is a powerful approach in which the material properties of a tunable platform are used to emulate user-defined model Hamiltonians. One of the biggest challenges in materials-based quantum simulation is understanding how to exactly map material-specific changes onto model parameters in a given Hamiltonian. Here, we study the electronic structure resulting from tailored quasi-1D atomic Cs chains constructed atom by atom, using scanning tunneling microscopy and spectroscopy with the aim to uncover how Cs adatoms on InSb can be used for quantum simulation. We study the dependence of the Cs-induced confined electronic states as a function of various parameters of the chain structure. We find that the lowest-level states can be well described by a 1D confinement potential, determined by the chain length, and that the critical parameter determining the depth of the attractive potential is the Cs density. We relate the observations to a lattice model Hamiltonian with exponential long-range hopping, and compare the calculated local density of states with the experimental observations, which reproduce the lowest energy states well. We find deviations from the 1D-confinement potential description for the higher-energy states, which we detail and speculate on its origin. These studies are critical for developing this material platform toward quantum simulation of electronic structure.

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## I. INTRODUCTION

Quantum simulation has become a viable route toward emulating the properties of model Hamiltonians that are often challenging to calculate both numerically and analytically. Using a variety of platforms, it has been shown that models like the Fermi-Hubbard model can be emulated in different limits [1–9]. The basis of quantum simulation is linking the material-specific properties of the simulator, and controllable changes of these, with a change in the parameters of the Hamiltonian that is being modeled. One of the challenges in these platforms is to emulate long-range hopping in the interacting limit within lattice models, to study, for example,  $t$ - $t'$ - $J$  models as needed to describe high-temperature superconductors [10–13].

Approaches using scanning tunneling microscopy/spectroscopy have become a viable platform for quantum simulation of electronic structure. It has been shown that individual atoms on surfaces can be bottom-up designed into one- and two-dimensional structures to study topology, Dirac Hamiltonians, as well as confined electronic structure in the single-particle limit [14–22]. To date, these approaches often rely on metallic surface states, which have extremely high carrier densities, leading to screening of electron-electron interactions and delocalization. Semiconductor surfaces have developed into a viable alternative, due to the inherently lower carrier density, compared to metal surfaces [23–26]. To this end, it was shown that Cs atoms on the surface of InSb(110) can be used to emulate atomic potentials and to realize atomic and molecular orbitals with multiorbital symmetry [27]. However, it is still not well understood how to map the material properties of such a platform and its tunability to parameters in an effective lattice Hamiltonian, such as the strength of a periodic potential and its hopping.

Here we experimentally construct and characterize quasi-1D chains derived from individual Cs atoms on the surface of InSb(110) as a model system to characterize the attractive potential formed by the Cs atoms and to investigate the resultant hopping. As previously reported, patterning individual Cs atoms on the InSb(110) surface creates an attractive potential due to their ionic nature after charge donation [27]. We found that atomic-size chains above a minimal length induce electronic states reminiscent of a 1D confinement potential. We characterized the changes in these electronic states, including

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the onset state energy (reflecting the depth of the potential) as well as the energy spacing between the higher-lying states. We found that the Cs density (i.e., the spacing between the Cs atoms) and the length of the chain are the key parameters in determining the attractive potential, by studying various structures including an alternating-spacing chain inspired by the Su-Schrieffer-Heeger (SSH) model. Furthermore, by investigating the spatial distribution of the local density of states (LDOS) for different states, we extracted an energy-dependent dispersion and relate this to the effective mass of the InSb conduction band. We developed a single-particle lattice model based on exponentially long-ranged hoppings. We found that we can quantitatively reproduce both the energy dispersion and the spatially dependent LDOS of the various states, using model parameters obtained from fits to the experimental data. Moreover, we found that higher-lying states of a given chain deviate from the confinement potential model. We detail these variations and discuss various possible sources, including a minimal model that considers additional subband contributions from the underlying two-dimensional electron gas (2DEG).

## II. EXPERIMENTAL METHODS

All experiments were performed using an Omicron low-temperature STM, operating in ultrahigh vacuum (UHV) and at a base temperature of  $T = 4.4$  K. Electrochemically etched W tips were used for all experiments, which were cleaned by electron-beam heating in UHV and field emission as well as dipped and characterized on clean Au(111). Undoped InSb(110) single crystals were cleaved in UHV conditions at room temperature and immediately transferred into the STM. Cs was subsequently evaporated onto the cold surface ( $T < 5$  K) [28]. Typical Cs densities were in the order of 0.005 monolayer (ML) (where one monolayer refers to one Cs atom per InSb(110) surface unit cell). Further details of the sample preparation can be found in Ref. [27].

Atomic manipulation was performed with typical tunneling parameters in the range of  $V_S = 12$ –20 mV and  $I_t = 50$ –300 pA with the feedback on. To assemble the Cs structures which lead to the formation of localized electronic states, we used lateral manipulation to move the Cs atoms. To this end, we first prepare our tip on a Au(111) surface by dipping and pulsing, until we have a stable and sharp tip which can resolve the spectroscopic features of the surface state on Au(111). Next, we prepare the tip on the InSb(110) surface by dipping and pulsing, until we can laterally manipulate Cs atoms. For details on the manipulation procedure, see Appendix A.

STS spectra were acquired after stabilizing the tip at  $V_S = 50$  mV,  $I_t = 100$  pA. No STS spectra were taken on top of atoms, as the use of typical stabilization parameters for STS resulted in the movement of atoms. The acquired line spectra were derived from sequences of STS spectra taken in constant-current mode, which were taken  $\sim 1$  nm above or below the long-axis of the chain. Spatially dependent maps of the differential conductance ( $dI/dV$ ) were acquired in constant-contour mode, as described in Refs. [27,29]. In these measurements, the contour traces were recorded at  $V_S = 200$  mV and  $I_t = 20$  pA, and then repeated at the bias voltage  $V$  of interest, with

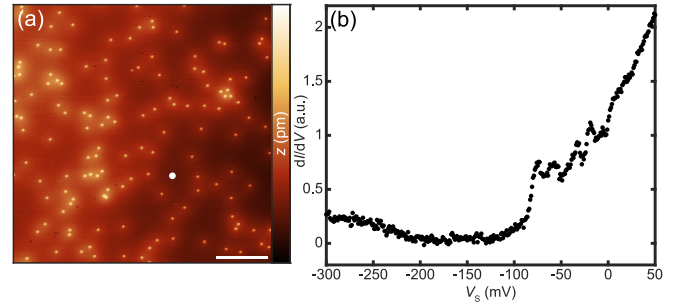


FIG. 1. (a) A constant-current STM image of the surface of InSb(110) after Cs deposition. The white dot indicates the position of the STS spectrum shown in (b) ( $V_S = 200$  mV,  $I_t = 20$  pA, scale bar = 20 nm). (b) An STS spectrum taken at the position indicated in (a) ( $I_{\text{stab}} = 100$  pA,  $V_{\text{stab}} = 50$  mV,  $V_{\text{mod}} = 1$  mV). In (a), a streak in the image caused by a tip change has been filtered.

$V_{\text{mod}} = 1$  mV (rms) and a constant  $z$ -offset of  $-140$  pm (i.e., closer to the surface). All maps shown were smoothed with a  $2 \times 2$  Gaussian filter.

## III. RESULTS AND DISCUSSION

### A. Bound state formation in short Cs chains on InSb(110)

The presence of Cs on the surface leads to downward band bending, pulling the conduction band below the Fermi energy ( $E_F$ ), which can be approximated by a triangular potential well in the  $z$  direction. This causes the formation of a 2D electron gas (2DEG) near the surface, as previously reported [29–32]. In Fig. 1(a), we show a typical coverage of Cs (0.004 ML) on the InSb(110) after deposition. Here, one monolayer (ML) is defined as one Cs atom per unit cell of InSb(110). The surface unit cell is defined by two orthogonal basis vectors:  $a_1 = 0.458$  nm is the InSb lattice spacing along  $[1\bar{1}0]$  (referred to as the  $x$  direction), and  $a_2 = 0.648$  nm is the InSb lattice spacing along  $[00\bar{1}]$  (referred to as the  $y$  direction). Individual Cs atoms are identified as individual bright protrusions on the surface. We also observe a small number of defects and impurities on the surface. We cannot readily identify the chemical composition of these various defects, although some are native to the bulk of the crystal, while others are residual surface contaminants, such as hydrogen. We note that large amounts of these impurities can also act as dopants on the bare InSb, as we have observed that this can introduce electronic disorder.

The onset of the 2DEG can be determined by taking STS at various locations on the surface and analyzing where the significant rise of conductance is within the band gap, appearing as a steplike feature. In Fig. 1(b) we show a typical STS spectrum on the disordered 2DEG of Cs/InSb(110). At  $V_S \approx -75$  mV we observe a steplike feature which we attribute to the onset of the first subband of the 2DEG. For this manuscript, we studied multiple samples where the 2DEG onset was located at voltages of approximately  $V_S = -100 \pm 25$  mV. The variance results from the local potential variation induced by the random distribution of Cs atoms. To minimize the hybridization between the induced electronic states of the 1D Cs structures and the electronic states arising from the background 2DEG, we laterally isolated the assembled

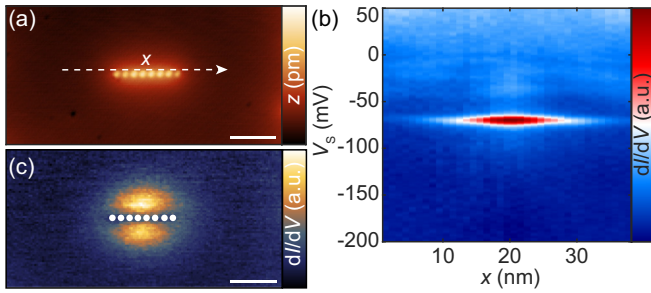


FIG. 2. (a) A constant-current STM image of a quasi-1D chain derived from eight Cs atoms along the  $[1\bar{1}0]$  direction on InSb(110) with an interatomic spacing of  $4a_1$  ( $V_s = 200$  mV,  $I_t = 20$  pA, scale bar = 10 nm). (b) False-color plot of  $dI/dV$  spectra taken along the dashed line indicated in (a) ( $I_{\text{stab}} = 100$  pA,  $V_{\text{stab}} = 50$  mV,  $V_{\text{mod}} = 1$  mV). (c) A constant-contour  $dI/dV$  map of the atomic chain taken at the bound-state energy of the chain ( $V_s \approx -75$  mV). The positions of the Cs atoms are indicated by added white circles in the image ( $I_{\text{tab}} = 20$  pA,  $V_{\text{stab}} = 200$  mV,  $V_{\text{mod}} = 1$  mV,  $z$ -offset =  $-140$  pm, scale bar = 10 nm).

structures by moving any unneeded Cs atoms typically 20 nm away from any assembled structure.

In Fig. 2, we illustrate the formation of a localized electronic state resulting from eight Cs atoms assembled into a single-atom width chain [Fig. 2(a)], with an interatomic spacing of  $a = 4a_1$  (referred to in the following as  $4a_1$  chain). STS spectra along the length of the chain near each Cs site [Fig. 2(b)], positions of the spectra marked by a dashed line in Fig. 2(a)] reveal a peak in  $dI/dV$  at  $V_s = -69 \pm 1$  mV, in the InSb bulk band gap, with maximum intensity at the center of the Cs chain. We extracted the energy by averaging over all spectra along the line and subsequently fitting a Lorentzian function to the averaged peak. The error is defined by the bias modulation of the lock-in amplifier. Using spatially dependent imaging [Fig. 2(c)], this state appears almost isotropic, similar to a bound  $s$ -like ground state for an individual artificial atom, as shown in Ref. [27]. The measured electronic state extends over approximately 11 nm from the edge of the chain in the  $x$  direction. We do not observe any corrugation in the LDOS

along the chain. This suggests that the potential variation induced by each individual Cs atom strongly overlaps with the adjacent atoms, leading to a potential well.

## B. Formation and length dependence of 1D electronic structure

In Fig. 3, we illustrate the effect on the confined electronic states when increasing the length of the chain ( $a = 4a_1$ ): for (a) 32 atoms, (b) 40 atoms, and (c) 48 atoms. Spectra taken along the length of each chain [Figs. 3(d)–3(f)] indicate the formation of a hierarchy of discrete states reminiscent of the properties of a particle in a square-well potential (commonly also referred to as a particle-in-a-box potential). To simplify the discussion, we assign a state number  $n$  to each state, starting with  $n = 1$  for the lowest state at the onset voltage  $V_1$ . As expected for a particle confined in a 1D potential, there is an increasing number of nodes and antinodes as the state index increases, as can be seen for all chains in Figs. 3(d)–3(f). Furthermore, as the chain length increases, going from 32 Cs atoms to 48 Cs atoms, the effective size of the potential well increases, leading to a smaller separation in energy between adjacent quantized states. The particle-in-a-box-like picture describes the hierarchy of states well up to a threshold voltage ( $V_{\text{thr}}$ ), which is approximately  $V_{\text{thr}} \approx -65$  mV. Above this, the discretized states show a more complex evolution, which we discuss later, in Sec. III F. In the subsequent discussion, we first focus on the spatial distribution of the states, as well as on the role of chain length and interatomic spacing on the electronic states.

The spatial extent of the confined states can be measured via constant-contour mapping [27].  $dI/dV$  maps of the four lowest discretized states at  $V_1$  to  $V_4$  for a  $4a_1$  chain consisting of 40 Cs atoms are illustrated in Figs. 4(a)–4(d). The maps reveal the expected structure of the LDOS, where the number of nodes increases with state index. Moreover, there is significant LDOS observed perpendicular to the chain, i.e., it is not completely localized within the structure of the Cs chain itself.

In addition to the spacing between the discrete states decreasing with increasing chain length, there is a trend for the energy of the onset state ( $E_1 = eV_1$ ) of the chain to decrease to

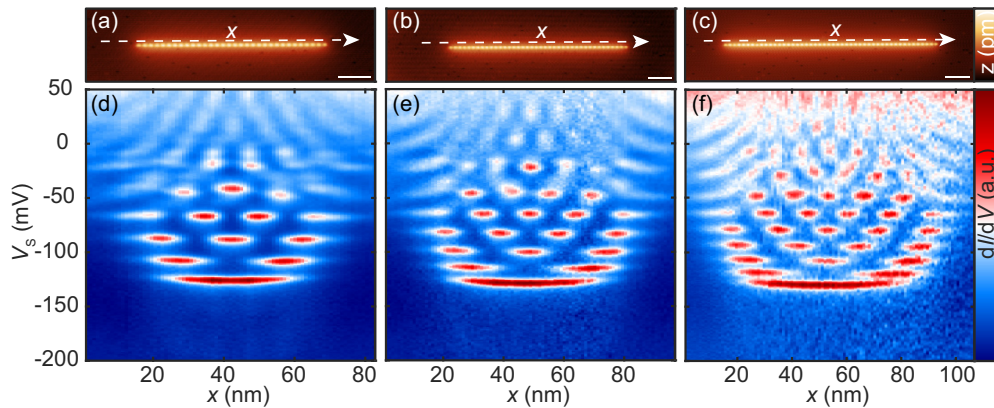


FIG. 3. (a)–(c) Constant-current STM images derived from quasi-1D chains with a  $4a_1$  spacing built from 32 Cs atoms with  $L \approx 56.8$  nm (a), 40 Cs atoms with  $L \approx 71.4$  nm (b), and 48 Cs atoms with  $L \approx 86.1$  nm (c) ( $V_s = 200$  mV,  $I_t = 20$  pA, scale bar = 10 nm). (d)–(f) False-color plots of  $dI/dV$  spectra along the chains, where the dashed arrows in (a)–(c) indicate the positions and directions of the spectra, respectively ( $I_{\text{stab}} = 100$  pA,  $V_{\text{stab}} = 50$  mV,  $V_{\text{mod}} = 1$  mV).

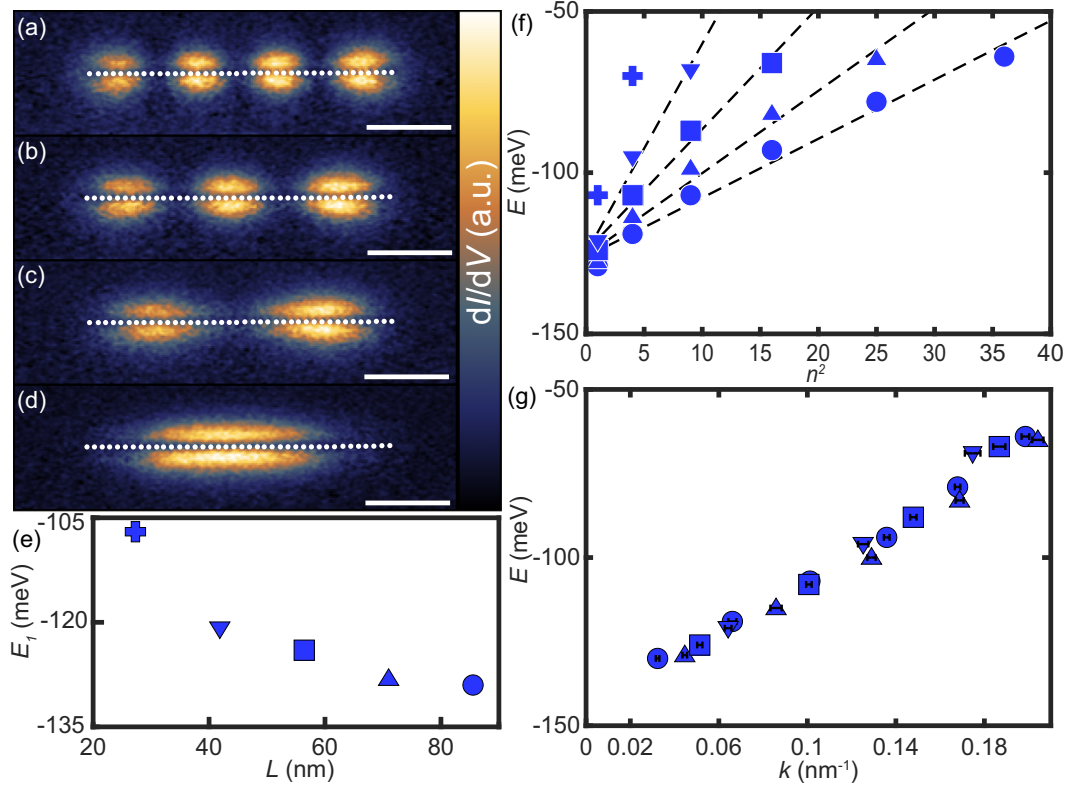


FIG. 4. (a)–(d) A set of constant-contour  $dI/dV$  maps of the quasi-1D chain with a  $4a_1$  spacing built from 40 Cs atoms shown in Fig. 3(b), taken at  $V_S = -83$  mV  $\approx V_4$  (a),  $V_S = -100$  mV  $\approx V_3$  (b),  $V_S = -115$  mV  $\approx V_2$  (c), and  $V_S = -129$  mV  $\approx V_1$  (d). The positions of the Cs atoms are indicated by added white circles in the image ( $I_{\text{stab}} = 20$  pA,  $V_{\text{stab}} = 200$  mV,  $V_{\text{mod}} = 1$  mV,  $z$ -offset =  $-140$  pm, scale bar =  $20$  nm). (e) Chain-length ( $L$ ) dependence of the energy  $E_1$  for the  $n = 1$  onset state for chains consisting of 16 (+), 24 ( $\nabla$ ), 32 ( $\square$ ), 40 ( $\Delta$ ), and 48 (O) atoms. The error in  $E_1$  of  $\pm 1$  meV is omitted for clarity. (f) Eigenvalues  $E_n$  of the chain states as a function of squared state index  $n^2$ , for chains consisting of 16 (+), 24 ( $\nabla$ ), 32 ( $\square$ ), 40 ( $\Delta$ ), and 48 (O) atoms. Dashed lines are parabolic fits,  $\alpha n^2 + \beta$ , for each chain length. The error in  $E_n$  of  $\pm 1$  meV is omitted for clarity. (g) Dispersion relation  $E(k)$  extracted from the spatial modulations of the eigenstates in the  $dI/dV$  maps, for chains consisting of 24 ( $\nabla$ ), 32 ( $\square$ ), 40 ( $\Delta$ ), and 48 (O) atoms. The error in  $E(k)$  of  $\pm 1$  meV is omitted for clarity. The error in  $k$  is given by four times the standard deviation of the fit used to extract  $k$ .

lower energy as the chain length increases. In Fig. 4(e),  $E_1$  is extracted as a function of chain length ( $L$ ), using the fitting procedure described in Sec. III A. The onset-state energy initially decreases with increasing chain length but quickly saturates and reaches an energy of  $E_1 = -129 \pm 1$  meV for the longest chains studied. Figure 4(f) summarizes the analysis of  $E_n$  vs  $n$  for all states identified below  $V_{\text{thr}}$  for five  $4a_1$  chains of different  $L$ . Each state index was fitted with a parabolic function (dashed lines), revealing a qualitative  $n^2$  dependence of  $E_n$ .

Although we are in the limit of discrete states, we can define a  $k$ -vector associated with the wavelength of the measured periodicity in the chain states as a function of chain length for a given spacing. We define  $k = 2\pi/\lambda$ , where  $\lambda$  is twice the distance between neighboring nodes (as  $\frac{dI}{dV}(x) \propto |\psi(x)|^2$ ). We note that for a finite square-well potential,  $k$  is not well defined and cannot strictly speaking be interpreted as a crystal momentum. Nevertheless, this approach allows us to compare the approximated dispersion relations  $E(k) = eV(k)$  for  $4a_1$  chains of different lengths with each other, which we present in Fig. 4(g). We find that all chains illustrate nearly the same dispersion, irrespective of their length, i.e., the chain length mostly defines the quantization condition but does not

strongly alter the imprinted 1D electronic structure. Moreover, the underlying effective mass of the conduction band, which is responsible for the electronic structure, does not strongly vary in the energy scales relevant for the chains. All of the above observations indicate that the lowest hierarchy of states can be described by a confined electron gas in a finite nearly square-well potential. We note that the edges of the well are not completely squarelike due to weak charge screening.

As the chain length further increases, a transition from a discrete hierarchy of states to a continuous band is expected. Figure 5(a) presents a  $4a_1$  chain built from 64 Cs atoms.  $dI/dV$  spectra taken along a line [Fig. 5(b)] reveal that the energetic spacing of the states is further reduced in comparison to chains of shorter length, to a degree where there is a significant spectral overlap of neighboring discrete states, which indicates the onset of band formation. In Fig. 5(c), we averaged all the spectra taken along the line. This averaged  $dI/dV$  spectrum does not show clear energy gaps, as can be seen for shorter chains [e.g., Fig. 3(d)], although oscillations can still be discriminated. We extract the energy difference between the  $n = 1$  and the  $n = 2$  state  $\Delta E_{12}$ , as a function of chain length ( $L$ ) for various  $4a_1$  chains [Fig. 5(d)]. This

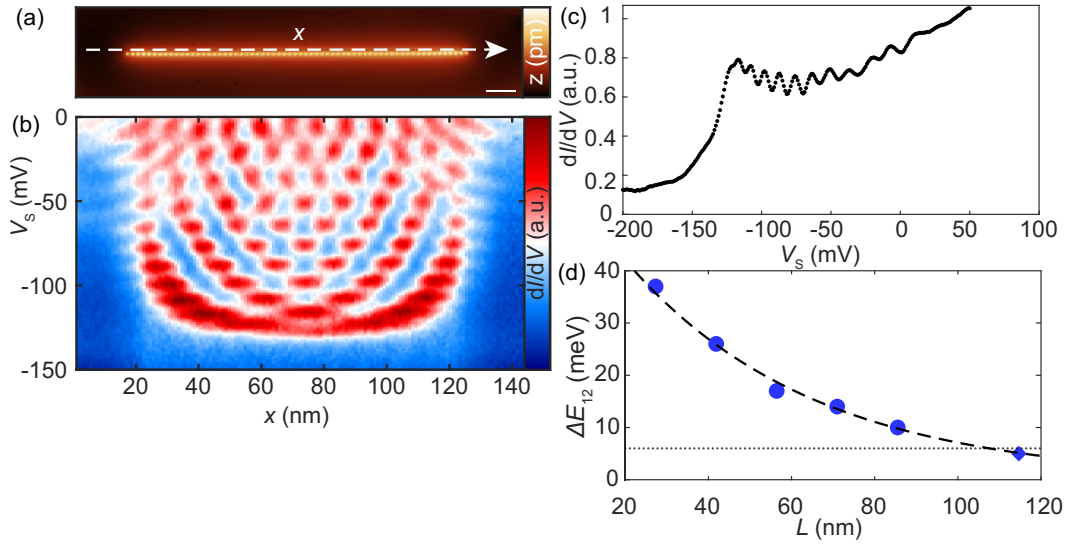


FIG. 5. (a) Constant-current STM image of a quasi-1D chain with a  $4a_1$  spacing built from 64 Cs atoms with  $L \approx 115$  nm ( $V_s = 200$  mV,  $I_t = 20$  pA, scale bar = 10 nm). (b) False-color plot of  $dI/dV$  spectra taken along the line marked in (a) ( $I_{\text{stab}} = 100$  pA,  $V_{\text{stab}} = 50$  mV,  $V_{\text{mod}} = 1$  mV). (c) Spatial average of all  $dI/dV$  spectra shown in (b). (d) Energy difference ( $\Delta E_{12}$ ) between the onset ( $n = 1$ ) and the second ( $n = 2$ ) state for various  $4a_1$  chains as a function of chain length, where the chain in (a) is marked as  $\diamond$ . The error bar in  $\Delta E_{12}$  of  $\pm 2$  meV is omitted for clarity. The curved dashed line serves as a guide to the eye. The straight dotted line marks the condition  $\Delta E_{12} = \Gamma/\sqrt{3}$ , assuming a width of  $\Gamma = 10$  meV (FWHM) for both the onset and the second state.

can be compared to the width  $\Gamma = 10 \pm 2$  meV (FWHM) that we find from Lorentz fits of all states below  $V_{\text{thr}}$ . As there is no local minimum present anymore in the superposition of two Lorentzians of equal width and amplitude when  $\Delta E_{12} \leq \Gamma/\sqrt{3}$ , we can estimate that the band limit is reached for a chain length  $L \approx 110$  nm. We note that the higher-order states below  $V_{\text{thr}}$  shown in Fig. 5(b) are still distinguishable, and a band formation across the full band width will therefore still require longer chains. As the widths of the states barely change with energy, the above condition for  $\Delta E$ , as illustrated in Fig. 5(d), also holds for the higher state separations. Nevertheless, this analysis is only a crude way of estimating the onset of band formation.

### C. Effect of interatomic spacing on 1D electronic structure

We subsequently explored the role of the interatomic spacing on the resultant confined states. In Fig. 6, we illustrate the constant-current images of two chains with similar length ( $L \approx 71$  nm) but different spacing: Fig. 6(a), a  $4a_1$  chain built from 40 Cs atoms, and Fig. 6(b), a  $5a_1$  chain with 32 Cs atoms. The spectra taken along the chain length are illustrated in Figs. 6(c) and 6(d), respectively. Focusing on the lowest hierarchy of states ( $V_s \leq V_{\text{thr}}$ ), the  $5a_1$  chain has a higher onset energy ( $E_1 = -101 \pm 1$  meV), accompanied by a reduced level separation as compared to the states of the  $4a_1$  chain. For the two lowest states specifically, the energy separation in the  $4a_1$  chain ( $\Delta E_{12} = 14 \pm 2$  meV) is larger than in the  $5a_1$  chain ( $\Delta E_{12} = 9 \pm 2$  meV). The qualitative shape and distribution of these states is otherwise very similar in both cases. The qualitative difference between the confinement potential defined by these two different cases is most likely determined by the local density of Cs atoms, which is larger in the  $4a_1$  chain. This leads to a larger attractive potential.

In Fig. 7 we compare  $dI/dV$  maps for the lowest five states of a  $5a_1$  chain and a  $6a_1$  chain, both being of similar length ( $L \approx 107$  nm) and thus possessing a different local Cs density. Comparing the lowest hierarchy of states shows that the spatial distributions of the eigenstates are nearly indistinguishable, despite their different eigenenergies [e.g.,  $E_1 = -104$  meV (f) vs  $-89$  meV (l)]. This is also true when comparing these features to a  $4a_1$  chain of similar length (not shown). Therefore, we can conclude that the eigenenergies of the lowest hierarchy of eigenstates of a chain can be tuned by the density of Cs atoms within the chain.

To quantify the effect of Cs density on the lowest hierarchy of states, we compared their eigenenergies as a function of the state index  $n$  for chains with different interatomic distances. Figure 8(a) shows  $V_n$  vs  $n$  for three chains with a similar total length: a  $4a_1$  chain with 48 atoms ( $L \approx 86$  nm), a  $5a_1$  chain with 40 atoms ( $L \approx 89$  nm), and a  $6a_1$  chain with 32 atoms ( $L \approx 85$  nm). All chains roughly follow the  $n^2$  dependence of the eigenstate energy that would be expected for a particle in a 1D potential, with the  $4a_1$  chain deviating the most. The deviations from the  $n^2$  dependence arise from the change in the dispersion of the 2DEG. At the energies near the 2DEG onset, the dispersion is nearly parabolic. At higher energies, it was shown that the dispersion of the 2DEG becomes more linear, causing the deviations from the  $n^2$  dependence [30]. For the  $5a_1$  and  $6a_1$  chains this effect is less obvious, since these chains extend over a smaller voltage range below  $V_{\text{thr}}$ . The similar curvatures further indicate that, in a simplified nearly free electron picture and when interpolated to the continuum limit, the quasiparticles possess similar effective masses irrespective of the chain density. Based on the description and assumptions mentioned in Sec. III B, we can also extract each state's momentum  $k$  and plot the dispersion relations for all chain densities (i.e., chain length) as shown

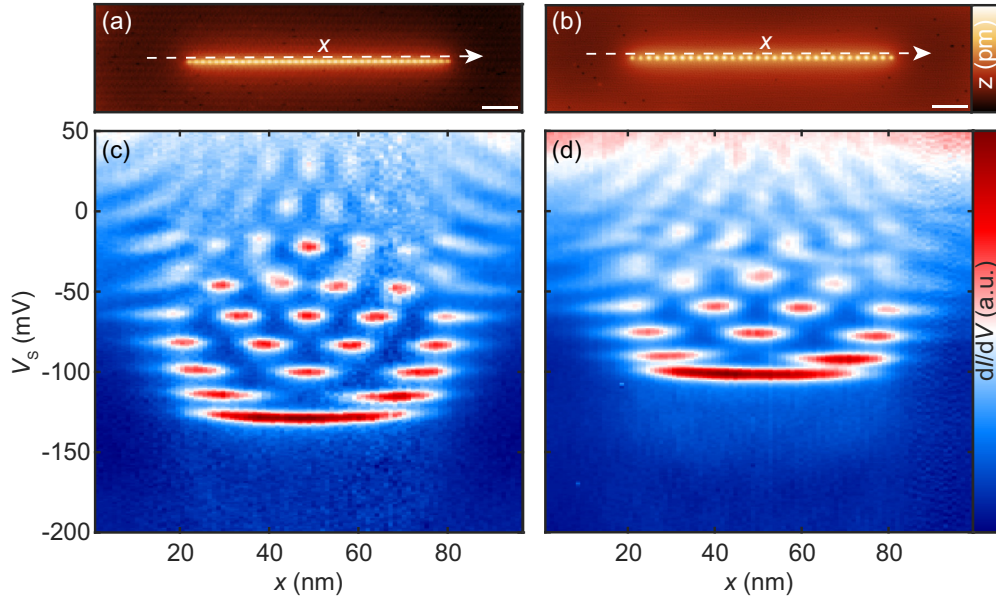


FIG. 6. Constant-current STM images (a), (b) and a false-color plot of a  $dI/dV$  spectra along a line (c), (d) of a quasi-1D chain derived from 40 Cs atoms with a spacing of  $4a_1$  (a), (c) and 32 atoms at a spacing of  $5a_1$  (b), (d). Both chains have a length of  $L \approx 71$  nm (imaging:  $V_s = 200$  mV,  $I_t = 20$  pA, scale bar = 10 nm); spectroscopy:  $I_{\text{stab}} = 100$  pA,  $V_{\text{stab}} = 50$  mV,  $V_{\text{mod}} = 1$  mV).

in Fig. 8(b). As was the case for the  $4a_1$  chains presented in Fig. 4(g), also the dispersions of all  $5a_1$  and  $6a_1$  chains follow the same dispersion, respectively, irrespective of the chain length. However, the dispersion relation clearly depends on the chain density. All dispersions tend to flatten roughly around their respective threshold voltages, which will be discussed later in Sec. III F. From Figs. 8(a) and 8(b) we can

roughly estimate an effective mass of  $m^* \approx 0.02 m_e$ . This compares well to the  $m^*$  value reported for the Cs/InSb(110) 2DEG in literature [32,33]. In the continuum limit, this would suggest that the effective mass is independent of the inter-atomic Cs spacing and is only determined by the value of the effective mass near the bottom of the conduction band of InSb(110).

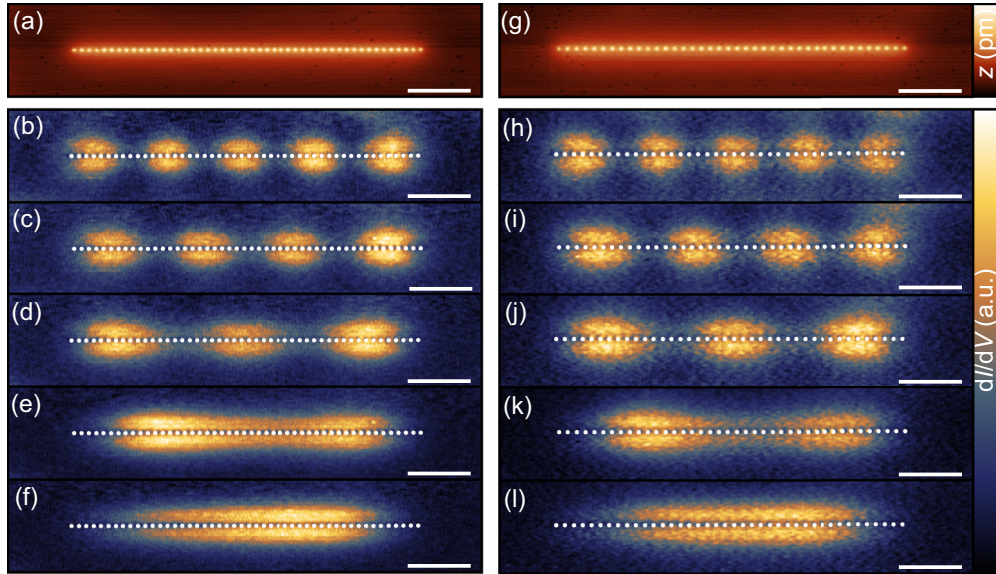


FIG. 7. (a) Constant-current STM image of a quasi-1D chain derived from 48 Cs atoms with a spacing of  $5a_1$ , i.e.,  $L \approx 107.6$  nm ( $V_s = 200$  mV,  $I_t = 20$  pA, scale bar = 20 nm). (b)–(f) A set of constant-contour  $dI/dV$  maps of the  $5a_1$  chain shown in (a), taken at  $V_s \approx -71$  mV (b),  $V_s \approx -82$  mV (c),  $V_s \approx -92$  mV (d),  $V_s \approx -100$  mV (e), and  $V_s \approx -104$  mV (f). (g) Constant-current STM image of a quasi-1D chain derived from 40 Cs atoms with a spacing of  $6a_1$ , i.e.,  $L \approx 107.2$  nm [same parameters as in (a)]. (h)–(l) A set of  $dI/dV$  maps of the  $6a_1$  chain shown in (g), taken at  $V_s \approx -54$  mV (h),  $V_s \approx -65$  mV (i),  $V_s \approx -75$  mV (j),  $V_s \approx -84$  mV (k),  $V_s \approx -89$  mV (l). The positions of the Cs atoms are indicated by white circles in each map ( $I_{\text{stab}} = 20$  pA,  $V_{\text{stab}} = 200$  mV,  $V_{\text{mod}} = 1$  mV,  $z$ -offset =  $-140$  pm; scale bar = 20 nm).

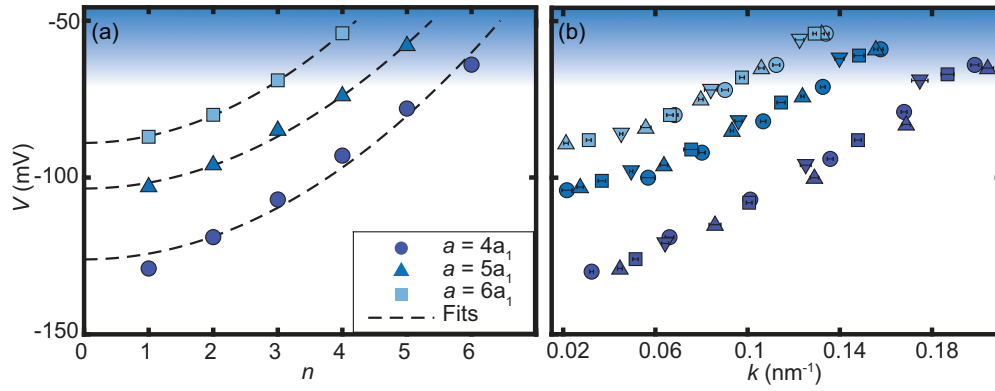


FIG. 8. (a) Voltages of the eigenstates vs their state index for quasi-1D chains derived from 48 Cs atoms (O) with a spacing of  $4a_1$  (dark blue), 40 Cs atoms ( $\Delta$ ) with a spacing of  $5a_1$  (medium-dark blue) and 32 Cs atoms ( $\square$ ) with a spacing of  $6a_1$  (light blue). The error bar in  $V$  of  $\pm 1$  mV is omitted for clarity. The dashed lines are quadratic fits,  $\alpha n^2 + \beta$ , through each set of states. The blue shaded area indicates the energies above the threshold ( $V_{\text{thr}} = -65$  mV) at which deviations are observed. (b) Dispersion relation  $V_n(k)$  extracted from the spatial modulation of the  $dI/dV$  maps, for chains with a spacing of  $4a_1$  (dark blue),  $5a_1$  (medium-dark blue), and  $6a_1$  (light blue), and consisting of 24 ( $\nabla$ ), 32 ( $\square$ ), 40 ( $\Delta$ ), and 48 (O) atoms. The error in  $k$  is given by four times the standard deviation of the fit used to extract  $k$ . The error in  $V$  of  $\pm 1$  mV is omitted for clarity. The blue shaded area indicates the energies above the threshold ( $V_{\text{thr}} = -65$  mV) at which deviations are observed.

#### D. Experimental evidence beyond nearest-neighbor hopping

Mapping the experimental system to an effective single-particle lattice model requires linking the physical parameters, such as the location of a Cs atom and its distance to its neighbors, to an effective on-site and hopping parameter. In the simplest limit, one can consider a one-orbital model defined by a nearest-neighbor hopping parameter. To ascertain whether only nearest-neighbor hopping is relevant, we constructed two chains built from 24 Cs atoms and with the same

total length of  $L \approx 42$  nm, but with different internal structure: (i) with a constant  $4a_1$  spacing [Fig. 9(a)], and (ii) with an alternating  $3a_1 - 5a_1$  spacing [Fig. 9(b)]. For only nearest-neighbor hopping, chain (i) can be described by one hopping parameter, whereas chain (ii) would require two hopping parameters, reminiscent of the SSH model [34]. In this limit, the hierarchy of states as well as their spatial distributions would be distinguishable between the two cases. The experimentally resulting electronic structure of these two cases is plotted in Figs. 9(c) and 9(d). The spectra for the two cases

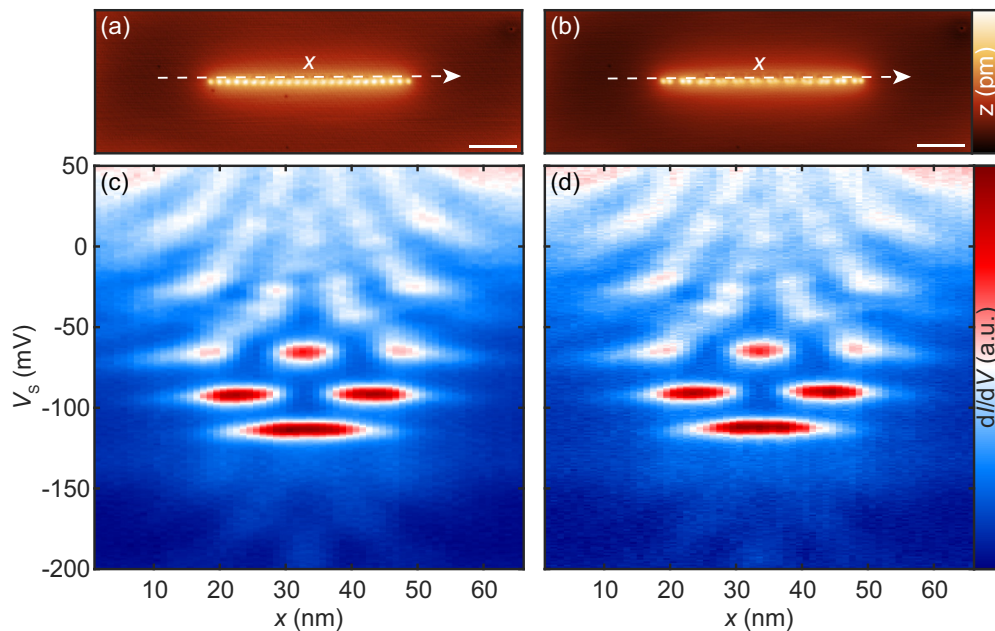


FIG. 9. Constant-current STM images (a), (b) and false-color plots of  $dI/dV$  spectra along a line (c), (d) of a quasi-1D chain derived from 24 Cs atoms with a spacing of  $4a_1$  (a), (c), and 24 atoms with a spacing alternating between  $3a_1$  and  $5a_1$  (b), (d). Both chains have a length of  $L = 42.1$  nm. The dashed arrows in (a), (b) indicate the positions and directions of the spectra (imaging:  $V_s = 200$  mV,  $I_t = 20$  pA, scale bar = 10 nm); spectroscopy:  $I_{\text{stab}} = 100$  pA,  $V_{\text{stab}} = 50$  mV,  $V_{\text{mod}} = 1$  mV).

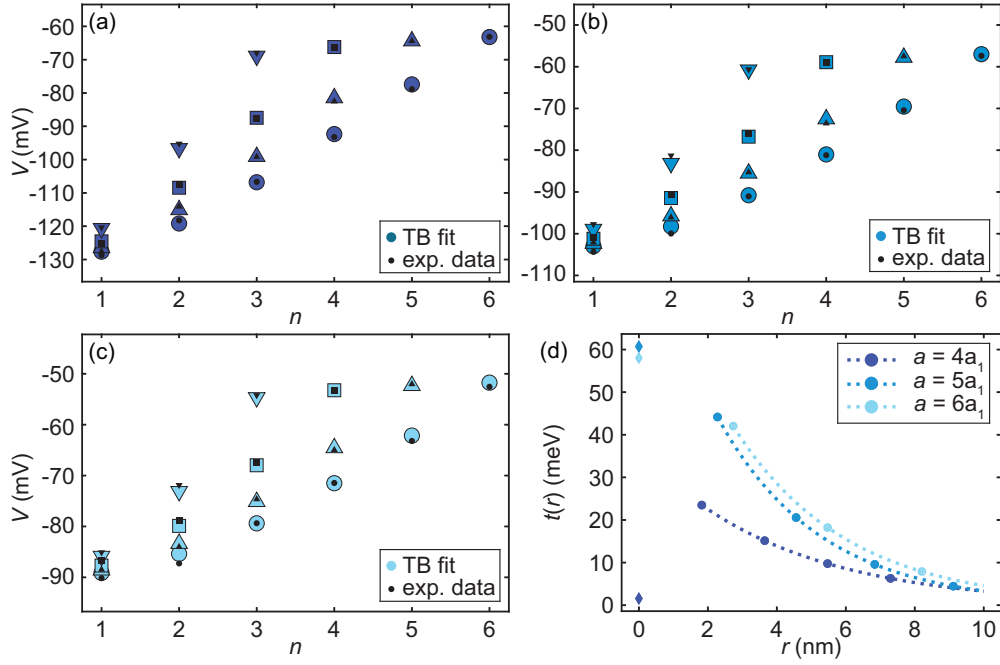


FIG. 10. (a)–(c) The calculated (colored), and the experimentally determined (black), energies ( $V$ ) of the lowest hierarchy of states as a function of the state index ( $n$ ) for quasi-1D chains derived from 48 Cs atoms (O), 40 Cs atoms ( $\Delta$ ), 32 Cs atoms ( $\square$ ), and 24 Cs atoms ( $\nabla$ ), with a spacing of  $4a_1$  [(a), dark blue],  $5a_1$  [(b), medium-dark blue], and  $6a_1$  [(c), light blue]. The error in  $V$  on the experimental data of  $\pm 1$  mV is omitted for clarity. (d) The distance-dependent hopping  $t(r)$  as a function of distance  $r$  for chains with a spacing of  $4a_1$  (dark blue),  $5a_1$  (medium-dark blue), and  $6a_1$  (light blue). The points at  $r = 0$  ( $\diamond$ ) indicate the on-site energy  $t_0$  which includes chemical potential shifts.

are nearly indistinguishable. The onset state energy of both chains ( $E_1 = -113 \pm 1$  meV) is nearly identical, as argued above, due to the nearly identical Cs density. The separations of the first two states ( $\Delta E_{12} = 23 \pm 2$  meV) and those of the second and third state ( $\Delta E_{23} = 26 \pm 2$  meV) are all the same for both chains. This is in stark contrast to the cases where the chain length or Cs density was varied, since the chain length and density affect the energy separation between the states and the Cs density affects the onset energy. The strong similarities of the electronic structures for the  $4a_1$  and the  $3a_1 - 5a_1$  chains thus show that we cannot fully describe the system within a solely nearest-neighbor hopping tight-binding-like model.

### E. Comparison between experiment and lattice model calculations

Before discussing how to model the resultant electronic structure, we note that the origin of the tailored electronic structure does not originate from the overlap of potential  $6s$  orbitals stemming from each Cs atom. The interpolated dispersion of the various structures suggests that the effective mass is spacing independent, for all structures, and comparable to the effective mass of the InSb conduction band. We moreover do not see any clear changes in this effective mass value for the SSH-inspired chains, which would be dramatically modified in a description relying primarily on nearest-neighbor hopping of electrons originating from bound  $6s$  states of Cs. Finally, we do not observe any clear signatures of an atomic  $6s$  state for an individual Cs atom, or bonding/antibonding states for a dimer of individual Cs states.

Therefore, we conclude that the origins of the interactions in the various structures studied stems from substrate-mediated interactions.

To rationalize our experimental findings in a model that goes beyond nearest-neighbor hopping, we construct a single-particle lattice Hamiltonian with spatially exponentially decaying hopping terms. Specifically, we introduce a long-range hopping between different sites  $i \neq j$  as  $t_{ij} = -\epsilon \cdot e^{-\alpha r_{ij}}$ , where  $\alpha$  is controlling the decaying length and  $\epsilon$  the hopping strength. For the on-site energy ( $i = j$ ) we define a third independent parameter  $t_0$  which includes chemical potential shifts. In analogy to atomic Wannier orbitals, we choose the position of every Cs atom of the chain to represent a lattice site hosting a single orbital in the model. The total form of the Hamiltonian is then

$$H = \begin{pmatrix} t_0 & t_{12} & t_{13} & \cdots \\ t_{21} & t_0 & t_{23} & \cdots \\ t_{31} & t_{32} & t_0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

Hence,  $\alpha$ ,  $t_0$ , and  $\epsilon$  serve as free parameters for fitting the model eigenenergies (as obtained from diagonalizing  $H$ ) to the experimental state energies. Fitting is performed separately for each chain density (i.e., interatomic spacing), but for a particular density the fit is applied to the complete experimental dataset, i.e., chains of various lengths. The atomic positions are taken from the experimental data. Figure 10 shows the resulting eigenenergies in direct comparison with the experimental values for  $4a_1$  chains (a),  $5a_1$  chains (b), and  $6a_1$  chains (c). Overall, we find an excellent quantitative

agreement between the model and our experimental results. The calculated distance-dependent hopping parameters for all three chain densities are presented in Fig. 10(d). In all cases, we find nonvanishing hopping elements far beyond nearest neighbors. Using a model that only includes on-site, nearest- and next-nearest-neighbor hopping does not allow for as accurate fits to the experimental energies. This is an intriguing finding, as it suggests that the underlying basis functions are rather spread out, which could be understood from relatively shallow attractive Cs-induced potentials in the InSb(110). Furthermore, this shows that only three (density-dependent) parameters allow to most adequately reproduce various chain lengths such that arbitrary chain lengths can likely be predicted from the model. In fact, using the  $4a_1$  fitting parameters, we can perfectly reproduce the experimental energies of the  $3a_1$ – $5a_1$  chain (not shown). Moreover, the hopping strengths for  $5a_1$  and  $6a_1$  chains are quite similar, while those of the  $4a_1$  chains are much smaller. We note that a different behavior between the  $4a_1$  and the  $5a_1/6a_1$  chains can already be observed in the experimentally derived dispersion relations for the three chain densities [Fig. 8(b)], where the  $5a_1$  and  $6a_1$  chains only show a rigid energy shift and (below  $V_{\text{thr}}$ ) a parabolic nearly free electron behavior, while the  $4a_1$  chains follow a seemingly different dispersion. In our model parameters this is reflected in a much smaller  $\alpha$ , such that the long-range hopping parameters are much less dependent on the distance, while the on-site element  $t_0$  is strongly suppressed. This is consistent with the interpretation that neighboring attractive Cs-induced potentials overlap more in the  $4a_1$  case such that an electron is less strongly bound to a single lattice site and therefore much more delocalized over the whole chain.

To also compare the spatial distribution of eigenstates between our experimental results and the model calculations, we applied a Green's function approach to calculate the energy and spatial dependence of the LDOS according to

$$\rho(r, \omega) = -\frac{1}{\pi} \text{Im } G(r, r, \omega)$$

with the Green's function

$$G(r, r', \omega) = \sum_{i,j} \phi_i(r) [(1(\omega + i\eta) - H)^{-1}]_{i,j} \phi_j(r')$$

for which we assume a Gaussian real-space  $s$ -orbital-like basis set  $\phi_i(r) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(r-r_i)^2}{2\sigma^2}}$  centered at the Cs positions and an energy broadening  $\eta$ . This way we can fit the experimentally observed spectral and spatial widths. We find that  $\sigma = 4$  and  $6$  nm (for  $4a_1$  and the  $5a_1/6a_1$  chains, respectively) and  $\eta = 4$  meV yield consistently good agreement with the experimental LDOS. The rather large  $\sigma$  is again in agreement with our assumption that the Cs-induced potentials are shallow such that the local basis functions are spread out. Note that these effective local basis functions have a much larger spatial extent than what one would expect for an atomic  $6s$  orbital of an isolated Cs atom. This demonstrates the role of the InSb(110) substrate in facilitating the long-range hopping. In Appendix B we show schematically how the physical system relates to measured electronic structure and how we relate this to the parameters in the lattice model.

Representative of all chains, the results for a  $4a_1$  chain with 40 Cs atoms are shown in Fig. 11, next to the corresponding experimental data for comparison. Below  $V_{\text{thr}}$ , the LDOS along the chain [Fig. 11(f)] is in excellent agreement with the experimental  $dI/dV$  spectra [Fig. 11(a)], reflecting both an increasing number of nodes with increasing state index and a slight overall decrease in LDOS intensity with increasing energy. The spatial extent of the states along the length of the chain also agrees well with the experimental findings. This is further manifested in the comparison of the experimental  $dI/dV$  maps [Figs. 11(b)–11(e)] with the calculated LDOS maps [Figs. 11(g)–11(j)] for the first four eigenstates ( $n=1$ – $4$ ), showing similar spatial extents of the antinodes in both  $x$  and  $y$  directions, including the fact that the wave functions do not extend much farther than the end of the chain.

### F. Higher-energy states and deviations from the effective single $s$ -orbital-like basis description

To this point, we primarily considered the lowest hierarchy of states below the threshold voltage ( $V_{\text{thr}}$ ), which can be described well by a single-particle lattice model with one  $s$ -like orbital and long-range hopping. At higher  $V_S > V_{\text{thr}}$ , we observe various deviations, namely the energy separations, the number of nodes, and the spatial distributions of the observed states do not continue the sequence observed for the lower-lying states. For example, the  $n = 5$  state of the  $4a_1$  chain built from 40 Cs atoms [Fig. 3(e)], which is located at  $V_S = -65$  mV, has the outer antinodes at the end of the chain spatially delocalized outward much farther than the states below  $V_{\text{thr}}$ . This enhanced delocalization is accompanied by a reduced LDOS intensity of the outer antinodes in comparison to the inner ones of the state located near the center of the chain. A similar trend can be found for the  $n \geq 4$  states of the 32-atom chain [Fig. 3(d)], the  $n \geq 6$  states of the 48-atom chain [Fig. 3(f)] as well as the  $n \geq 9$  of the 64-atom chain [Fig. 5(b)]. Moreover, additional states can be identified above  $V_{\text{thr}}$  that do not follow the expected trend of linear increasing number of nodes with increasing state number. We note that the value of  $V_{\text{thr}}$  may be dependent on the spacing, but we typically observe deviations for  $V_{\text{thr}} \approx -60$  mV and above.

To illustrate the deviations, we present  $dI/dV$  maps of the  $4a_1$  chain with 40 Cs atoms at four distinct voltages above  $V_{\text{thr}}$  [Figs. 12(b)–12(e)] and replot the line spectra for reference in Fig. 12(a). The spatial distribution of each of these states does not strictly follow the trend of a successively increasing number of nodes with increasing state number. For example, the map in Fig. 12(c) shows an eigenstate with only three nodes, although the eigenstates below [Fig. 12(d)] and above [Fig. 12(b)] possess five and six nodes, respectively. In general, the antinodes are also not equidistantly distributed and there is a general increase in  $dI/dV$  intensity orthogonal to the chain direction, reminiscent of a contribution of another orbital type. Furthermore, the LDOS intensity of the antinodes for a given state is no longer equal, but the nodes closer to the ends of the chain are weaker [Figs. 12(b), 12(d), 12(e)]. The antinodes at the ends of the chain extend much further outward along the  $x$  direction. This was already visible in the  $dI/dV$  spectra taken along a line [Fig. 12(a)], but is also confirmed in the maps [Figs. 12(b), 12(d), 12(e)].

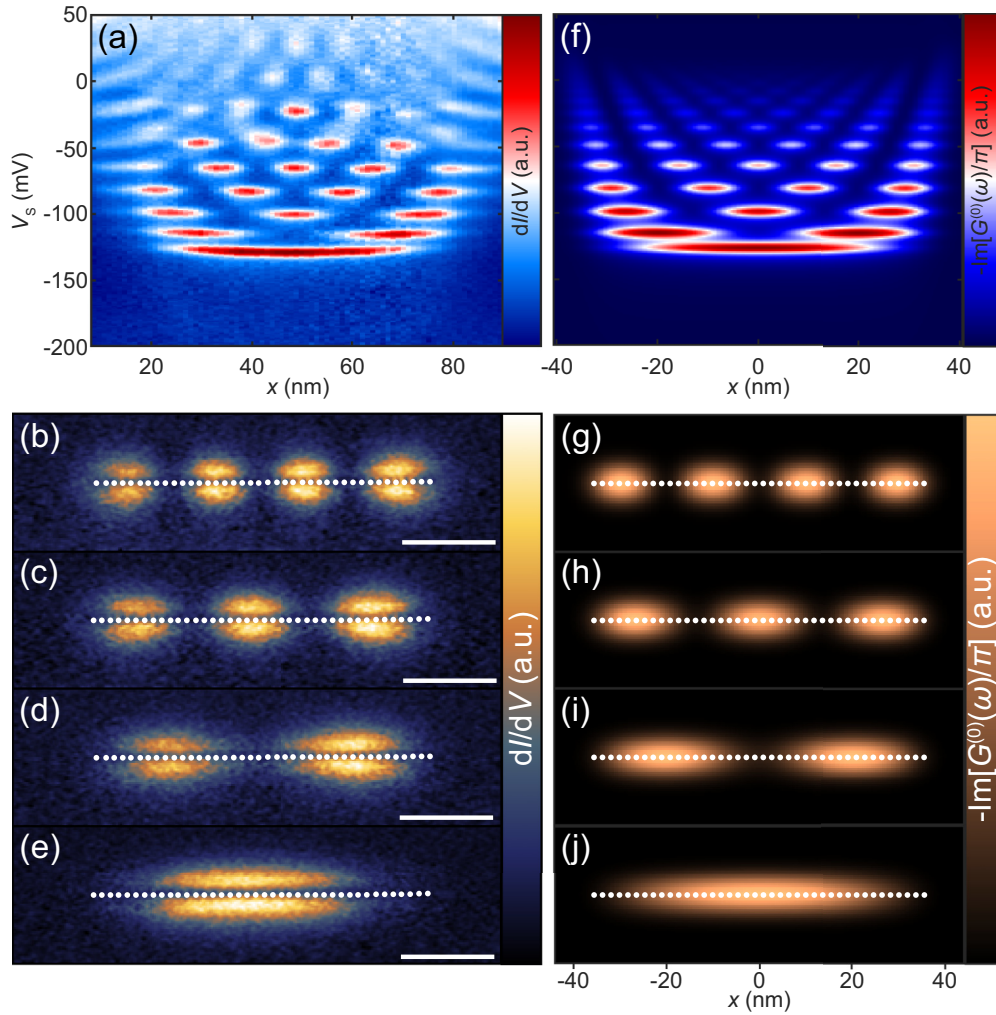


FIG. 11. (a) False-color plots of  $dI/dV$  spectra along a quasi-1D chain derived from 40 Cs atoms with a spacing of  $4a_1$  (cf. Fig. 3). (b)–(e) A set of constant-contour  $dI/dV$  maps of the chain in (a) taken with  $V_s \approx -83$  mV (b),  $V_s \approx -100$  mV (c),  $V_s \approx -115$  mV (d), and  $V_s \approx -129$  mV (e). The positions of the Cs atoms are indicated by added white circles in the image: ( $I_{\text{stab}} = 20$  pA,  $V_{\text{stab}} = 200$  mV,  $V_{\text{mod}} = 1$  mV,  $z$ -offset =  $-140$  pm, scale bar = 20 nm). (f) A false-color plot of the calculated spectra of the same chain using a lattice model with long-range hopping. (g)–(j) A set of plots of the calculated real-space LDOS of the lowest four states in (f) at the energies  $V = -82$  meV (g),  $V = -99$  meV (h),  $V = -112$  meV (i),  $V = -127$  meV (j). The positions of the atomic sites are indicated by added white circles in the plot.

We contemplate several possible origins for these deviations. First, we discuss the role of tip-induced band bending (TIBB), which is typically relevant in III–V (110) surfaces. In Appendix C we investigate the effects of TIBB, by measuring the electronic structure of the same  $4a_1$  chain with two different stabilization parameters (i.e., two different tip-sample separations). In general, we do not observe strong TIBB [30], presumably due to the metallic nature of the 2DEG, which may partially screen the tip electric field. We thus conclude that the observed deviations above  $V_{\text{thr}}$  are not caused by TIBB.

With relation to the increased intensity seen orthogonal to the chain, one can consider the contributions of another orbital state. It was previously found that artificial atoms derived from rings of Cs atoms can host  $p$ -like states at higher voltages [27]. The chain's geometry breaks the degeneracy between potential  $p_x$  and  $p_y$  orbitals such that the onset of potential  $p_y$  states would be significantly lower in energy. In this way, the increased intensities in the  $dI/dV$  maps above and below

the chain in Figs. 12(b)–12(e) may stem from extended  $p_y$ -like states, which energetically overlap with the  $s$ -like states discussed so far. We note that, based on the geometry and symmetry of the chain,  $sp$ -hybridization is unlikely, and therefore this cannot explain the shape of the LDOS distributions we measure. Moreover, the onset of  $p_y$  states and the spacing between these states should be dependent on the chain density and length, akin to the  $s$ -like states (e.g., Fig. 6). However, we found that the onset of deviations ( $V_{\text{thr}}$ ) described above occur at a relatively fixed energy, independent of the chain length. This suggests that we may rule out the role of a second orbital state in the chain itself.

Another consideration could be the shape of the attractive potential at higher energy, namely the shape of the potential is not necessarily squarelike at all energies. For the lowest states, the attractive potential can be approximated in the square-well limit. However, at higher energies, due to interplay between band bending and screening, the attractive potential toward the end of the chain structure will bend to equilibrate the poten-

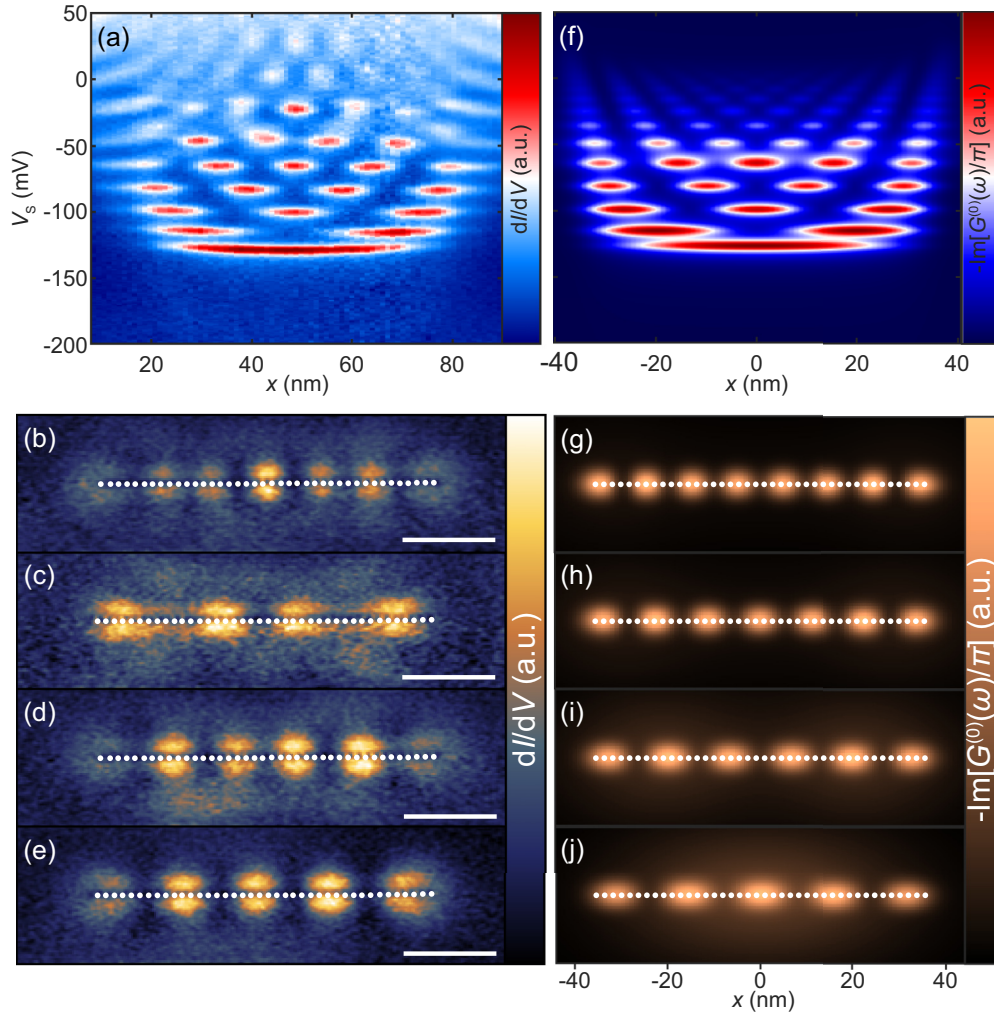


FIG. 12. (a) False-color plots of  $dI/dV$  spectra along a quasi-1D chain derived from 40 Cs atoms with a spacing of  $4a_1$  (cf. Fig. 3). (b)–(e) A set of constant-contour  $dI/dV$  maps of the chain in (a) taken at  $V_S \approx -27$  mV (b),  $V_S \approx -37$  mV (c),  $V_S \approx -47$  mV (d) and  $V_S \approx -65$  mV (e). The positions of the Cs atoms are indicated by added white circles in the image: ( $I_{\text{stab}} = 20$  pA,  $V_{\text{stab}} = 200$  mV,  $V_{\text{mod}} = 1$  mV,  $z$ -offset  $= -140$  pm, scale bar  $= 20$  nm). (f) A false color plot of the calculated line spectrum of the same chain using a long-range hopping model incorporating the localization of both the first and second 2DEG. (g)–(j) A set of plots of the calculated real-space LDOS of four states in (c) at the energies  $V = -25$  meV (g),  $V = -36$  meV (h),  $V = -49$  meV (i),  $V = -64$  meV (j). The positions of the atomic sites are indicated by added white circles in the plot.

tials between the surrounding 2DEG and the chain structure. This will lead to a variation from a squarelike well along the axis of the chain. In the simplest limit, this will lead to LDOS that is allowed to leak outside of the chain, when compared to the square-well limit. We cannot rule out that this has a contribution to the measured spatially dependent LDOS of the higher-energy states.

It is also important to consider that the effective potential created by the Cs structures is not truly 1D in nature. The tailored potential also has a component along the axis orthogonal to the chain axis. This can lead to an additional quantization axis, which can introduce a second index reminiscent of a rectangular 2D confinement potential (e.g., state numbers  $n_x$  and  $n_y$ ). In this picture, the eigenstates below  $V_{\text{thr}}$  would then all be indexed with  $n_y = 1$ , and additional states with  $n_y = 2$  might exist above  $V_{\text{thr}}$ . However, if there is an additional subband introduced at  $V_{\text{thr}}$ , this sets a lower bound on the energy difference between the eigenstates introduced by the

second quantization axis. This therefore could only explain the contribution of an additional state. However, we see more complex variations in the  $y$  direction as a function of energy on a smaller energy scale. Therefore, the expected confinement potential in the  $y$  direction is most likely not solely responsible for the variations we observe.

The final consideration we make originates from the underlying 2DEG itself, which is coupled to the chain. In the simplest approximation, we can consider the band bending that yields the 2DEG as a triangular confinement potential along the  $z$  direction. It was previously shown that this confinement potential can host a second 2DEG subband, which is typically located 50–80 meV above the first subband, depending on the InSb bulk doping as well as the Cs concentration [29–32]. It is therefore possible that there is an onset of a second set of confined states, that may overlap with the confinement states from the first 2DEG subband. In order to consider the influence of this second subband,

we modeled the influence of such a second 2DEG in our model calculations by assuming that the Cs atoms in the chain induce localized states within the second 2DEG in a similar way as for the first 2DEG, but at a higher energy. Hence, these states are less bound, and as such the  $s$ -like orbitals are spatially and energetically more spread out (we set  $\sigma_2 = 5\sigma$  and  $\eta_2 = 2\eta$ ). The results of these calculations are shown in Figs. 12(f)–12(j). In our calculations, this leads to a second set of 1D confinement states that are spatially broader and energetically closer-spaced. If we assume that these sets of induced states do not interact with each other, such that the resulting Hamiltonian is block-diagonal, we can simply add their spectral weights and LDOS and obtain the results presented in Fig. 12(f). Comparing to the results from Fig. 11(f), the lowest set of states is not affected, since they are below the onset of the second set of confinements states. However, there is an additional state right around  $V_{\text{thr}}$ , between the  $n = 5$  and  $n = 6$  states of the first set of confinement states. We also can reproduce the fact that the antinodes of the eigenstates above  $V_{\text{thr}}$  do not anymore have equal intensity but are more pronounced in the center of the chain, which is simply an effect of superposition of the two sets of eigenstates. Looking into the calculated spatial maps, [Figs. 12(g)–12(j)] we find additional LDOS along the  $y$  direction off the chain [Figs. 12(i) and 12(j)], which qualitatively explains this type of feature in the experimental maps.

There are, however, several features that cannot be reproduced by this minimal model. Most notably, the additional state with less nodes [Fig. 12(c)] cannot be explained. Also, the significantly weaker antinodes at the chain ends [Figs. 12(b) and 12(d)] and the strikingly enhanced central antinode in Fig. 12(b) are not reproduced by the model. Furthermore, the second set of confinement states with  $n \geq 2$  quickly loses spectral weight and is barely visible in the model, hence it barely modifies the first set of confinement states in the superposition. Therefore, we cannot rule out that there are additional contributions or that the second subband is solely responsible for the deviation behavior we detail. For instance, it may be possible that the two sets of confinement states can interact with each other, that the artificial electronic structure hybridizes with the surrounding 2DEG of the Cs/InSb(110) surface, or that many-body excitations may need to be considered.

#### IV. CONCLUSION

In conclusion, we constructed and characterized the electronic states derived from quasi-1D atomic chains derived from Cs atoms on the surface of InSb(110). We used these chains as a model system to study the role of Cs in creating an attractive potential that can be used for quantum simulation. With this we found quantum dotlike properties for very short chains built from eight Cs atoms, and showed the onset of 1D behavior that, below a particular threshold voltage, is reminiscent of the properties of a particle in a 1D potential well for chains with  $\geq 16$  Cs atoms. We studied the dependence of the confined states as a function of chain length and chain spacing. Above a certain chain length, the energy of the first eigenstate merely changes with chain length, and the underlying dispersion relation is the same for all chains, the length

only determining the confinement condition. Reducing the interatomic distance leads to a deeper confinement potential and modifies the dispersion relation. By defining an effective dispersion using the periodicity of the LDOS, we found that the dispersion of states is roughly determined by the effective mass of the bottom of the conduction band of InSb. We also found that the Cs density is the driving parameter in determining the depth of the attractive potential, whereas the length of the chain structure determines its width. In this limit, atomic-scale variations play a smaller role. The latter was evidenced by constructing a uniform chain and comparing its electronic structure to a dimerization-inspired chain, which showed nearly identical electronic structure. We demonstrated by mapping the material system to a single-particle lattice model that the electronic properties of these chains exhibit significant long-range hopping. We specifically showed that the hopping can be described by an exponential term  $t_{ij} = -\epsilon \cdot e^{-\alpha r_{ij}}$ . Using a Green's function approach in combination with  $s$ -like Wannier orbitals centered at the Cs positions, we compared the real-space LDOS with the measured STS maps of the lowest-energy confined states and find excellent agreement. This suggests that the attractive potential formed from individual Cs atoms is shallow, and that in the chain structure studied, these potentials strongly overlap, leading to long-range hopping far beyond nearest neighbors.

In addition to describing the lowest states, we also observed significant deviations from the expected well potential-like description for higher-energy states in various chains. We found that the onset of these deviations occurs above a threshold voltage, which was relatively insensitive to the geometry of the chain. After considering various sources, we focused on a possible additional set of confinement states derived from a second 2DEG subband, which may be superimposed with the higher-energy states of the first set. As this can only explain some of the deviations, we suggest that hybridization effects between the subsets or even with the surrounding 2DEG generated by the Cs atoms on the surface may play a role, requiring further future investigation. This study allows for a more precise mapping between the Cs structures created experimentally and a lattice model. This is imperative in order to use such a platform for quantum simulation of electronic structure and ultimately understanding the role of interactions that lead to wave functions that cannot be described in the single-particle limit.

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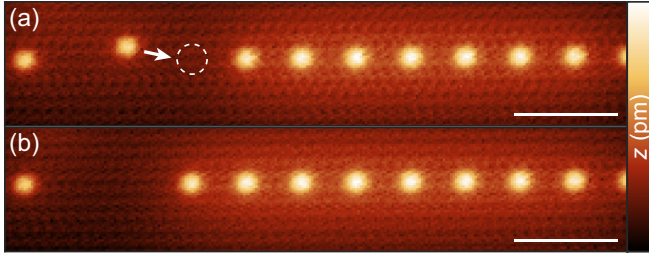


FIG. 13. Two subsequent constant-current STM images demonstrating the construction of a quasi-1D chain of Cs atoms with a  $6a_1$  spacing. (a) The chain before extending it with one Cs. The white arrow indicates the direction of the lateral manipulation. The white circle indicates the position where the atom is left ( $V_S = 200$  mV,  $I_t = 20$  pA, scale bar = 5 nm). (b) The chain after the extension with one Cs ( $V_S = 200$  mV,  $I_t = 20$  pA, scale bar = 5 nm).

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manuscript. All authors participated in discussions about the scientific interpretation of the results. In addition, the first three authors equally contributed to the manuscript, and the order of these equally contributing authors was alphabetically chosen.

## DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

## APPENDIX A: ATOMIC MANIPULATION DETAILS

To be able to manipulate Cs atoms, we prepare the tip on the InSb(110) surface by dipping and pulsing, until we can laterally manipulate Cs atoms. A typical lateral manipulation event involves three steps: (i) Approach the tip on top of the Cs, (ii) move the tip laterally while the Cs follows the tip, and (iii) retracting the tip slightly and moving laterally off the Cs. The approach starts from  $V_S = 200$  mV and  $I_t = 20$  pA and ends at  $V_S = 12 - 20$  mV,  $I_t = 50 - 300$  pA, where the precise parameters depend on the tip. At the final parameters the Cs will follow the tip as it is moved laterally. To leave the Cs on the surface, the tunneling current is reduced to  $I_t = 20 - 50$  pA and the tip is moved in the  $[00\bar{1}]$  or  $[001]$  direction. In Fig. 13, we show the extension of a Cs chain ( $6a_1$  spacing) by one Cs. The Cs atom in Fig. 13(a) is moved along the trajectory indicated by the arrow. Subsequently the atom is left in the position of the white circle. In Fig. 13(b) we show the subsequent image where the Cs is now incorporated into the chain.

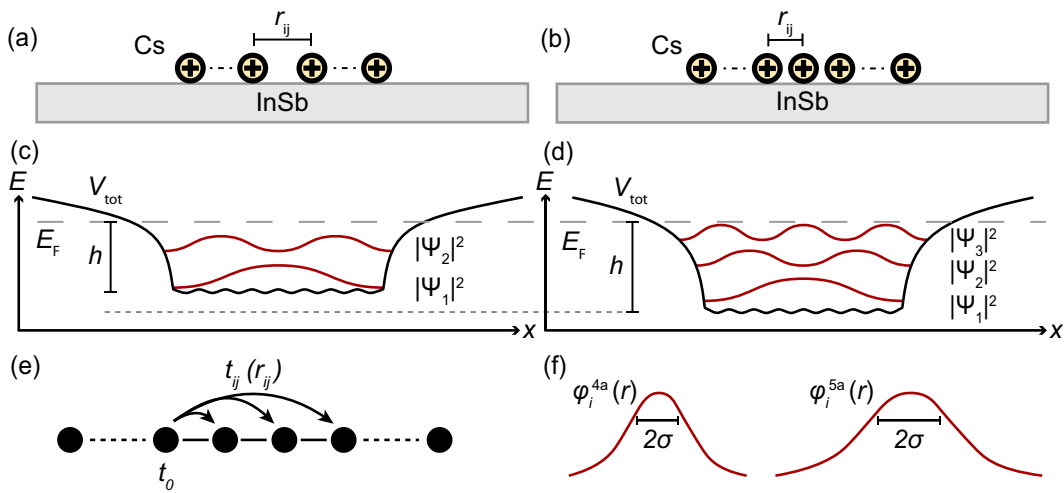


FIG. 14. (a), (b) Schematic representation of two different Cs chains. The distance between two individual Cs atoms is given by  $r_{ij}$ . (c), (d) A schematic depicting the potential ( $V_{\text{tot}}$ ) with a depth ( $h$ ) induced in the InSb(110) by the Cs chains in (a) and (b), respectively. The part of the potential below the Fermi energy ( $E_F$ ) gives rise to occupied electronic states with a probability density ( $|\Psi_n|^2$ ). (e) A schematic of the corresponding lattice model. Every dot depicts a site in the lattice model with an on-site energy parameter ( $t_0$ ). The long-range hopping parameter ( $t_{ij}$ ) between two sites is a function of the distance between the Cs atoms ( $r_{ij}$ ). (f) A schematic of the Gaussian basis functions ( $\phi_i(r)$ ). The parameter  $\sigma$  determines the spatial width of the basis function.

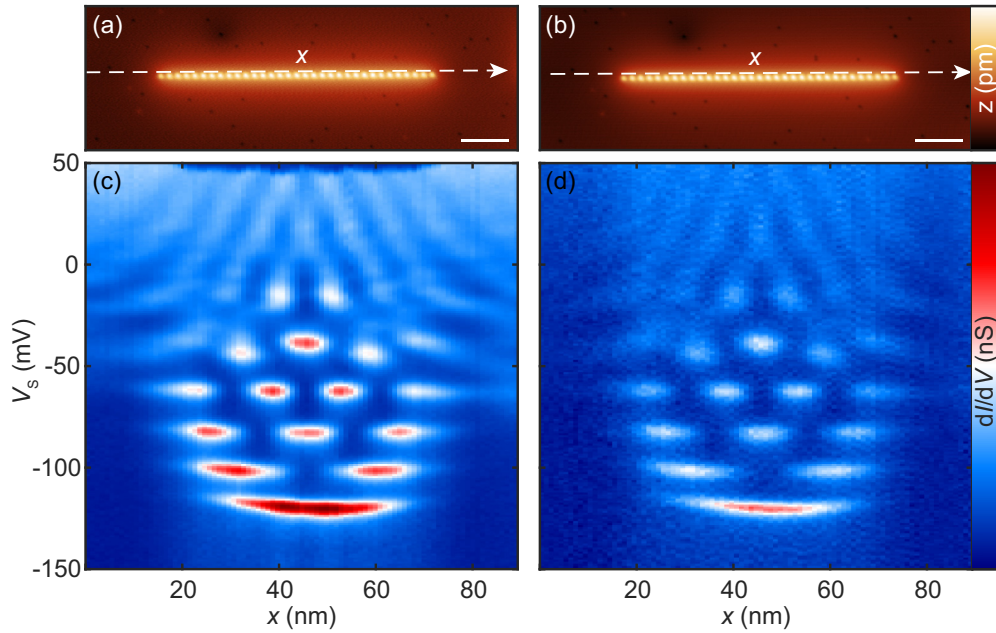


FIG. 15. Constant-current STM images (a), (b) and false-color plots of  $dI/dV$  spectra along a line (c), (d) of the same quasi-1D chain derived from 33 Cs atoms with a spacing of  $4a_1$ . The dashed arrows in (a), (b) indicate the positions and directions of the spectra in (c), (d). The spectra in (c), (d) are taken at different stabilization parameters but are plotted with the same color scale. The tip-sample distance in (d) is approximately 200 pm larger than in (c) (imaging:  $V_S = 200$  mV,  $I_t = 20$  pA, scale bar = 10 nm; spectroscopy: (c)  $I_{\text{stab}} = 100$  pA,  $V_{\text{stab}} = 50$  mV,  $V_{\text{mod}} = 1$  mV and (d)  $I_{\text{stab}} = 200$  pA,  $V_{\text{stab}} = 350$  mV,  $V_{\text{mod}} = 1$  mV).

## APPENDIX B: RELATION BETWEEN THE PHYSICAL SYSTEM, ITS ELECTRONIC STRUCTURE, AND THE LATTICE MODEL

In order to obtain the parameters in the lattice model, we need to be able to relate this to parameters in the physical system. In Fig. 14, we show how the parameters in the physical system relate to the measured electronic structure. We then subsequently connect this to parameters in the lattice model which reproduce the same electronic structure. We consider two different chains of Cs atoms. The chain in Fig. 14(a) has a lower Cs density than the chain in Fig. 14(b). The potential induced in the InSb(110) surface by the Cs atoms is shown in Figs. 14(c) and 14(d), corresponding to the chains in Figs. 14(a) and 14(b), respectively. The depth of the potential is larger for the denser chain due to the higher Cs concentration. The part of the potential below Fermi level gives rise to occupied electronic states. Figure 14(e) depicts the corresponding lattice model, where the position of every Cs atom corresponds to a site in the lattice model. The long-range hopping term then depends on the distance ( $r_{ij}$ ) between the sites. The real space LDOS can be calculated using a

Green's function approach. Figure 14(f) shows the Gaussian real-space basis set used in this approach. The spatial width of the basis functions is smaller for chains with a  $4a_1$  spacing compared to chains with a  $5a_1$  or  $6a_1$  spacing.

## APPENDIX C: ABSENCE OF EFFECTS FROM TIP-INDUCED BAND BENDING

Tip-induced band bending (TIBB) is a common phenomenon in III-V semiconductors. To evaluate whether TIBB is a possible cause of the deviations observed at higher energies, we measured the same  $4a_1$  chain with two different stabilization parameters (i.e., different tip-sample distances), as shown in Fig. 15. Qualitatively, the measured electronic structure is identical for the smaller [Fig. 15(c)] and the larger [Fig. 14(d)] tip-sample distance, the only difference being a decrease in  $dI/dV$  intensity for the latter. Hence, we can exclude TIBB to play a relevant role in our experiments, and we conclude that the deviations above  $V_{\text{thr}}$  must have a different origin.

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