**I. INTRODUCTION**

For the past two decades, quantum transport properties of atomic scale conductors have received great attention both experimentally and theoretically\(^1\) since they present the ultimate size limit of functional electronic devices and have great potential utilities in molecular electronic devices. However, previous investigations on these atomic scale conductors were primarily concentrated on molecules or atomic lines, etc. Less attention has been focused on the electrical transport properties of clusters. They suggested that Ge\(_n\) clusters are the magic number clusters, both theoretically and experimentally\(^1\), since they present the ultimate size limit of functional electronic devices and have great potential utilities in molecular electronic devices. Therefore, it is of fundamental and practical importance to investigate the transport behavior of clusters, especially of those magic number clusters, both theoretically and experimentally.

Among all these clusters, the group-IV semiconductor clusters have received intensive theoretical and experimental\(^1\) investigations for the past two decades since they have fundamental importance and potential applications in nanoelectronics. Therefore, the geometrical and electronic structure properties of small germanium clusters are already well understood. In particular, the experimental measurement of the mass spectra\(^1\) of Ge\(_n\) clusters has shown that Ge\(_4\), Ge\(_7\), Ge\(_{10}\), Ge\(_{14}\), Ge\(_{16}\), and their cations are magic number clusters, which are geometrically and electronically stable. Theoretically, Wang’s and co-workers\(^5\) have performed density-functional electronic structure calculations on the Ge\(_n\) (\(n=2–25\)) clusters. They suggested that these Ge\(_n\) clusters are more stable than their neighboring clusters.

Specifically, their calculated results showed that the ionization potentials are extremely high at \(n=7\) and 10 and that Ge\(_7\) and Ge\(_{10}\) clusters are the most stable species. Consequently, in the current work we take the cluster Ge\(_7\) with enhanced stability as an example to perform our *ab initio* investigations of the transport properties of the clusters since it is expected that more stable clusters are more advantageous to the experimental observation.

For the transport properties of the group-IV semiconductor clusters, to the best our knowledge, there has been no report about Ge\(_n\) clusters so far. However, for Si\(_n\) clusters, an *ab initio* calculation has been performed by Roland et al.\(^1\) In their theoretical calculations, the ultrathin silver nanowires along the same orientation (001) and the same cluster-electrode separation are adopted for most clusters. Their calculations showed that under small voltages, all of the clusters display metallic current-voltage (I-V) characteristics and that the typical conductances range between 2 and 3 \(G_0\) (\(G_0=2e^2/h\), conductance quantum). At the same time, taking the smallest three magic clusters Si\(_4\), as an example, we have also systematically probed the effect of contact geometry and gating on the transport properties of silicon clusters. In most of current theoretical investigations of the molecular conductors so far, the metallic nanowires have been often chosen as the atomic scale electrodes for the calculation, especially those along the crystal direction [100]. However, based on the experimental indication, Ag, Au, and Cu nanowires (Refs. 25–27) along [110] are the most frequently observed among the three crystal directions [100], [110], and [111]. Moreover, Hong et al.\(^1\) have successfully obtained ultrathin single-crystalline silver nanowires, with 4 Å width and only four atoms in the cross section. Hence, besides the atomic scale electrodes along [100] as generally used in most current calculations, the ultrathin silver nanowires along [110] are also adopted as model electrodes in our theoretical calculations.
Furthermore, it is well known that the metallic nanowires (MNW’s) have been of great interest as building blocks for the nanoelectronic devices. Therefore, besides the investigations of transport properties of the Ge7 cluster in contact with the above two kinds of atomic scale silver electrodes along [110] and [100], we also probe the transport properties of these two perfect MNW’s composed of these two kinds of electrodes, respectively. The theoretical calculations are based on the combination of density-functional theory (DFT) with a nonequilibrium Green’s function (NEGF) technique.29,30 Our results show that under strong cluster-electrode coupling, the equilibrium conductance of the Ge7 cluster connected to thin Ag wires takes the value of about 3 and 4 Ge7 in the case of Ag(110) and Ag(100), respectively, and that there exists a close correlation between the electronic structure of the electrodes and the transport properties of this cluster. At the same time, the geometric and electronic structure properties of the Ge7 cluster have also been calculated. Our results present that the ground state of the Ge7 cluster is a pentagonal bipyramid with \( D_{5h} \) symmetry and that the highest occupied molecular orbital (HOMO)-lowest unoccupied molecular orbital (LUMO) gap is 1.75 eV, which agrees well with previous work.7 The HOMO orbital is a \( \sigma \)-type bonding orbital composed of dominant \( s \) and \( p_z \) components on the pentagon germanium atoms, and the LUMO is an antibonding orbital consisting of \( s \) and \( p_z \) components on all germanium atoms.

This paper is organized in the following way: the computational method and the device model are briefly described in Sec. II, the results and discussions are presented in Sec. III, and a short summary is given in Sec. IV.

II. CALCULATION METHOD AND SIMULATION MODEL

The calculations have been carried out by using the program TRANSISTERA-TATK), which is based on the combination of DFT (as implemented in the well tested SIESTA method31 with the NEGF technique.29,30 The TRANSISTERA-TATK package is able to model the electrical properties of nanoscale devices without inducing phenomenological parameters. These nanoscale devices, which are referred to as two-probe systems, consist of an atomic scale system coupled with two semi-infinite electrodes, as shown in Fig. 1. In practical theoretical simulations, such a two-probe system is divided into three parts: the left electrode, the right electrode, and the central scattering region. The scattering region actually includes a portion of the semi-infinite electrodes. Details of the method and relevant references can be found elsewhere.32,33 The current through this atomic scale system is calculated from Landauer-Büttiker formula34

\[
I(V_b) = \frac{2e}{h} \int_{\mu_l}^{\mu_r} dT(E, V_b),
\]

(1)

where \( \mu_l \) and \( \mu_r \) are the electrochemical potentials of the left and right electrodes, respectively, for an applied bias \( V_b \).

\[
\mu_l(V_b) = \mu_l(0) + eV_b/2,
\]

(2)

\( T(E, V_b) \) is evaluated by the transmission coefficients \( T(E) \) at the Fermi energy \( E_F \) of the system

\[
G = \frac{2e^2}{h} T(E_F).
\]

(5)

In our first-principles calculations, the local-density approximation to the exchange-correlation potential, specifically, the functional of Perdew and Zunger,36 is used. Only valence electrons are considered in the calculation, and the wave functions are expanded by localized numerical (pseudo)atom orbitals.37 The atomic cores are described by norm-conserving pseudopotentials.38 The convergence criterion for the Hamiltonian, charge density, and band-structure energy is \( 10^{-4} \) via the mixture of the Hamiltonian.

The two-probe structural models for our theoretical calculation are illustrated in Fig. 1, in which a Ge7 cluster is symmetrically coupled with two kinds of atomic silver nanowire electrodes Ag(100) and Ag(110). The fivefold axis of the Ge7 pentagonal bipyramid is along the z direction. For simplicity, these two-probe systems are respectively referred to as Ge7-Ag(100) and Ge7-Ag(110). These two kinds of nanowires are both built by alternately stacking the bulk [100] or [110] atomic layers, and the structures are both labeled as \( n/m \), where \( n \) is the atom number taken from one layer and \( m \) is the atom number taken from the other. For the [110] nanowire electrode, the structure 4/1 is adopted and

FIG. 1. (Color online) The two-probe geometry of the Ge7 cluster connected with two kinds of silver nanowire electrodes: (a) the Ag(100) case, in which the atomic arrangement of the corresponding nanowire electrode is 4/5; and (b) the Ag(110) case, in which the atomic arrangement of the corresponding nanowire electrode is 4/1. The contact distances \( d1 \) and \( d2 \) are the vertical distances between the germanium atom on the fivefold axis in the Ge7 pentagonal bipyramid and the corresponding surface of the surface-atom layers, respectively.

\[
\mu_l(V_b) = \mu_l(0) - eV_b/2.
\]

(3)

For simplicity, the \( \mu_l(0) \) and \( \mu_r(0) \) are set to zero. The energy region between \( -eV_b/2 \) and \( +eV_b/2 \), which contributes to the current integral above, is referred to as the bias window. \( T(E, V_b) \) is the transmission coefficient at energy \( E \) and bias voltage \( V_b \). Based on the eigenchannel decomposition of the conductance, this total transmission \( T(E) \) can be decomposed into nonmixing eigenchannels \( T_n(E) \) (Ref. 35) as

\[
T(E) = \sum_n T_n(E).
\]

(4)
4/5 is used for the [100] case. In our investigations, these atomic Ag nanowires have been chosen as ideal electrode models without geometry optimization, as generally adopted in most current theoretical calculations about molecular conductors. In these two adopted models, a large enough vacuum layer is included for the electrode cell in the x and y directions so that the device has no interaction with its mirror images, and four and six silver atomic layers have been chosen for the electrode cell in the z direction for the Ge7–Ag(100) and Ge7–Ag(110) systems, respectively. In the central region of these two structural models, several atomic layers in the left and right electrodes, which are denoted as surface-atom layers, are chosen to screen the perturbation effect of the cluster on the Kohn-Sham potential outside the scattering region. For the system Ge7–Ag(100), the surface-atom layers of the left (right) are three (four), and they are five (six) for the Ge7–Ag(110), as indicated by the two vertical lines in the Figs. 1(a) and 1(b).

III. RESULTS AND DISCUSSIONS

A. Determination of cluster-electrode distance

As we all know, the conductor-electrode distance is an important parameter, but it is difficult to precisely measure and control in the present experiments related to the molecular conductance. In the previous work about the transport properties of the Si6 cluster, the cluster-electrode contact distance is 4.215 a.u., in which one of silicon clusters takes the maximum equilibrium conductance. In our present investigations, the contact distance is determined by the equilibrium distance between one germanium atom and the corresponding silver surface obtained via the total-energy calculation as follows. A five-layer slab with a (2×2) unit cell has been chosen to model the Ag(100) and Ag(110) surfaces, and one germanium atom is placed above the hollow surface site, which has been proved to be the most energetically favorable. The vertical distance between this germanium atom and the slab is then varied and the total energy of the whole adatom-slab system is evaluated. The obtained total energy as a function of the Ge-slab vertical distance is shown in Fig. 2. This figure shows that the nearest cluster-surface vertical distance is 1.50 and 1.12 Å, corresponding to the nearest-neighbor distances \( d_{Ge-Ag} \) of 2.54 and 2.75 Å in the case of Ag(100) and Ag(110), which agree well with those of the previous work (2.60 and 2.70 Å) for the Ag(100) and Ag(110), respectively. Thus, these obtained vertical distances are chosen to be the cluster-electrode contact distances between the germanium atom of the fivefold axis in the Ge7 pentagonal bipyramid and the corresponding surface of the surface-atom layers. Correspondingly, these distances are the strong-coupling bonding distances for the Ge7 cluster and electrodes. In order to systematically probe the transport properties of this cluster, we have also considered other contact distances.

B. Transport properties under zero bias

Based on the method described in Sec. II, we firstly probe the equilibrium transport properties of the Ge7 cluster, which is symmetrically sandwiched between two kinds of silver electrodes, and perfect infinite silver nanowires composed by these atomic scale electrodes, respectively. In Fig. 3, the transmission spectra of the perfect silver nanowires and the Ge7 cluster are both presented for the Ag(100) and Ag(110) cases. For clarity, the Fermi level has been shifted to \( E_F = 0 \). As for these two infinite pure nanowires, the transmission spectra \( T(E) \) are both step functions. In the case of Ag(100) nanowire presented in Fig. 3(a), the equilibrium conductance is 5 \( G_0 \), which means five conductance channels opening at the Fermi level and contributing to the total transmission. However, in the Ag(110) case shown in Fig. 3(b), the equilibrium conductance takes the value of 4 \( G_0 \), which implies there are four channels with contribution to the total transmission at the Fermi level. Thus, the difference in the equilibrium conductance for these two kinds of nanowires is 1 \( G_0 \). Moreover, Fig. 3(a) also presents that the \( T(E) \) curve of Ag(100) nanowire exhibits a sharp steplike increase and that the transmission probability quickly increases from 2 to 6 \( G_0 \) in a small energy region between −0.3 and +0.3 eV. However, the \( T(E) \) spectrum varies smoothly and the transmission probability only increases from 3 to 4 \( G_0 \) in the above energy region near the Fermi level in the case of Ag(110). For the Ge7 cluster, it takes the equilibrium conductance of 3.76 \( G_0 \) when it is placed between two Ag(100) electrodes, whereas the equilibrium conductance is 2.92 \( G_0 \) in the Ag(110)-electrode situation. Accordingly, we notice that for the same cluster, the conductance difference under these two kinds of
electrodes composed by the same element is close to 1 $G_0$. Most importantly, the overall curve shape of the $T(E)$ spectrum of the cluster closely follows that of the corresponding infinite nanowire in these two cases, as shown in Fig. 3, which is similar to the behavior of metallic impurities in thin Cu nanowire reported by Papanikolaou et al.\textsuperscript{41} Corresponding to the variation in the transmission spectra of the pure nanowires, in the above small energy region from −0.3 to +0.3 eV, the transmission spectrum of the Ge$_7$ cluster coupled with the electrode Ag(110) changes smoothly and the value only alters from 2.5 to 3.0 $G_0$. However, the transmission probability of this cluster in contact with the Ag(100) electrodes quickly increases from −1.0 to 4.0 $G_0$ in this small energy region.

As for such a close transmission curve shape following between the Ge$_7$ cluster and the corresponding nanowire, it is necessary and interesting to probe if the Ge$_7$ cluster does play an active role in the Ge$_7$-Ag(100) and Ge$_7$-Ag(110) systems. Therefore, we take away the Ge$_7$ cluster from these Ge$_7$ two-probe systems while keeping the distance between the left and right electrodes [5.84 and 5.09 Å for the Ge$_7$-Ag(100) and Ge$_7$-Ag(110) systems, respectively] unvaried, then perform calculations on these systems to investigate the direct tunneling from one electrode to the other. For simplicity, these two systems in which there only exist two electrodes are referred to as gap-Ag(100) and gap-Ag(110), respectively. The obtained results are shown in Fig. 3. In contrast to the transmission from the pure Ag nanowires and Ge$_7$ cluster, we clearly find that the direct tunneling through the left and right electrodes is very small in both gap-Ag(100) and gap-Ag(110) cases. Especially in the gap-Ag(100) case, the transmission is close to zero in a large energy region from −1.20 to −0.20 eV, and the equilibrium conductance is only 0.015. For the gap-Ag(110) system, the equilibrium transmission is 0.18, which is only 6% of the corresponding Ge$_7$-Ag(110) system. In fact, such a close spectra shape following can be understood as follows. When one Ge$_7$ cluster is placed between two electrodes and strongly coupled with these electrodes, there exist strong bonds between the cluster and electrodes, and the discrete energy levels of the isolate cluster will be much broadened and shifted.\textsuperscript{23,42} Consequently, these broadened and shifted energy levels might form a quasicontinuous energy-level distribution between the left and right electrodes. As a result, via such quasicontinuous energy levels, electrons can transmit from one electrode to the other as that in the pure silver nanowires, and thus the transmission spectra of the Ge$_7$ cluster are very smooth and do not display evident tunneling peaks, as presented in Fig. 3. However, once the cluster is taken away, there exist no broadened levels; it will be difficult for the electrons to directly transmit from one electrode to the other, and eventually the direct tunneling from one electrode to the other is small because the large separation

![Figure 3](image1)

**FIG. 3.** The total equilibrium transmission spectra of the Ge$_7$ cluster, together with the corresponding perfect silvers nanowires and the two-probe systems without Ge$_7$ cluster: (a) for the (100) case and (b) for the (110) case. The energy is relative to the Fermi level (vertical line).

![Figure 4](image2)

**FIG. 4.** The eigenchannel decomposition of the total equilibrium transition of the Ge$_7$ cluster around the Fermi level in the case of these two kinds of electrodes: (a) for the Ag(100) electrode and (b) for the Ag(110) electrode.
between the left and right electrodes. Therefore, as for the whole shape of the transmission spectra curve, such a close shape following indicates that the equilibrium transport properties of the Ge$_7$ cluster are closely related to the band structure of the nanowire electrodes when the cluster is strongly coupled with the electrodes. However, as for the weak coupling case, the energy levels of the conductors in the central region are less broadened and the electrons transmit, in principle, via resonant tunneling, and therefore there exist obvious tunneling peaks in the transmission spectra, as presented by Lee et al.,$^{24}$ where the transport properties of the atomic wire two-probe systems are more closely related to the isolated atomic chain itself.

To gain more insight into the transport properties of the Ge$_7$ cluster, we perform eigenchannel decomposition of the total transmission spectra of the cluster around the Fermi level, as shown in Fig. 4. There are five channels around the Fermi level contributing to the total transmission for the Ag(100) electrodes [Fig. 4(a)]. Among these channels, channels $T_1$ and $T_2$ are degenerate and open at about $E = -0.2$ eV. Once opened, the transmission probabilities of these two channels rapidly saturate to unity. Channel $T_5$ opens at around $E = -0.15$ eV and the transmission through this channel also increases rapidly in a very small energy region. In the case of Ag(110) shown in Fig. 4(b), it is observed that there are only four channels with contribution to the total transmission near the Fermi level. Among these channels, channel $T_1$ is always saturated to unity around the Fermi energy, and channel $T_4$ opens at $E = -0.25$ eV. Therefore, the Ge$_7$ cluster exhibits enhanced conductivity when it is coupled with the Ag(100) electrodes since more channels contribute to the total transmission at the Fermi level. In order to further probe the transport properties of the Ge$_7$ cluster, we then carry out band-structure calculations for these two infinite silver nanowires, as shown in Fig. 5. In the case of Ag(100) shown in Fig. 5(a), there are five electronic bands going across the Fermi level. The number of bands crossing the Fermi level is identical with the number of the conductance channel of the Ge$_7$-Ag(100) system and the Ag(100) infinite nanowire. Among these crossing bands, bands $b_1$ and $b_2$ are degenerate and stay at $\sim -0.2$ eV at the $\Gamma$ point, which correspond to the degenerate conductance channels $T_1$ and $T_2$, as shown in Fig. 4(a). For the Ag(110) case shown in Fig. 5(b), four bands are found to cross the Fermi level, in which band $b_1$ contributes to channel $T_4$, as presented in Fig. 4(b). Therefore, the number of bands crossing the Fermi level is also similar to the channel number of the Ge$_7$-Ag(100) system and the corresponding Ag(100) nanowire. As a result, for both the Ge$_7$ cluster and the infinite nanowire, our calculations imply that the number of conductance channels is determined by the number of electronic bands crossing the Fermi level. In the case of Ag(100) electrode, more bands crossing the Fermi level lead to more channels contributing to the total transmission around the Fermi energy, and eventually both the infinite nanowire and the Ge$_7$ cluster exhibit larger transmission conductance in the case of Ag(100) than in the Ag(110) case. Hence, when the cluster is strongly coupled with the electrodes, there exists a close correlation between the band structure of the electrode and the equilibrium transport properties of the Ge$_7$ cluster under different kinds of electrodes. However, the total conductance value of the cluster connected to Ag nanowires is determined by both the choice of the electrodes and the cluster itself, since the number of eigenchannels is that of electrode bands crossing the Fermi level but the transport probability through each channel is closely related to the cluster itself and its coupling with the electrodes.

Since the distance is difficult to precisely measure and control in the current experiments about the molecular conductance, to systematically probe the transport properties of the Ge$_7$ cluster, we have also investigated the equilibrium conductance of the Ge$_7$ cluster connected to Ag nanowires as a function of the cluster-electrode contact distance.

![FIG. 5. The band structure of the infinite perfect silver nanowires around the Fermi energy: (a) the Ag(100) nanowire and (b) the Ag(110) nanowire.](image)

![FIG. 6. The total equilibrium conductance of the Ge$_7$ cluster coupled with different electrodes as a function of the cluster-electrode contact distance.](image)
conductance under different cluster-electrode contact distances. The evolution of the equilibrium conductance with the contact distance is presented in Fig. 6 for both the Ge7-Ag(100) and Ge7-Ag(110) systems. As can be observed in this figure, the conductance variations present a similar trend for these two kinds of electrodes. However, the conductance of Ge7 coupled with the Ag(100) electrodes is larger than that in the case of Ag(110) electrodes under most of investigated distances. An oscillatory behavior of the equilibrium conductance exists in both situations. When the varied distances decrease from 4.0 to 1.0 Å, the conductance increases and reaches a local maximum at 2.8 and 2.4 Å firstly, then decreases until a local minimum appears at 2.6 Å for the Ge7-Ag(100) and Ge7-Ag(110) cases, respectively. The conductances turn to increase as the distances decrease further in both cases. Such a striking oscillatory behavior of the equilibrium conductance has also been found in other systems such as the Si4 cluster23 and Au atomic wires.24 This effect of contact distances on the transport properties can be understood from the cooperation or competition between the variation of the cluster-electrode coupling and the shift of energy level of the cluster as illustrated in our previous work in detail.23

C. Transport properties under finite bias

In Fig. 7, we display the calculated I-V curves of the Ge7 cluster in contact with silver electrodes. From this figure, it is clear that for both the Ag(110) and Ag(100) electrodes, the Ge7 cluster presents nonlinear I-V characteristics in the whole investigated voltage region. In particular, the Ge7 cluster displays metallic I-V characteristics in the bias voltage region between 0.0 and 1.2 eV in the case of Ag(110), but it exhibits metallic characteristics in a smaller region from 0.0 to 0.3 eV in the Ag(100) case. As shown in Eq. (1), the current in the system is calculated by the Landauer-Büttiker formula, which is transmission spectra dependent. In order to discuss such a different I-V behavior, we take the bias of 0.6 eV as an example to analyze the transmission difference under these two kinds of electrodes. Figure 8 presents the transmission curve of the Ge7 cluster for these two different kinds electrodes with the bias voltage being 0.6 eV. The bias window, which contributes to the current integral in the Landauer-Büttiker formula, is from −0.3 to 0.3 eV according to Eqs. (1)−(3). As in the case of Ag(100) electrodes shown in Fig. 8(a), the whole bias window can be divided into four regions. The first region is from −0.3 to 0.1 eV, in which there are only two eigenchannels contributing to the total transmission. The total transmission is close to 1.2 in this region. In the second one, from 0.1 to 0.15 eV, there exist four eigenchannels with contribution to the total transmission after two degenerate channels opening at ≈0.1 eV. For the third one, from 0.15 to 0.20 eV, the total transmission is contributed by five eigenchannels, in which channel T1 closes at ≈0.20 eV. The last one is from 0.20 to 0.30 eV, in which four channels contribute to the total transmission, and the transmission spectra display a platform with the total probability being ≈3.4 in this region. In the last three regions, there always exist two degenerate channels, especially in the last two regions, where these two degenerate channels have great contribution to the total transmission. At the same time, the whole bias window of the Ge7-Ag(110) system can also be divided into two regions. One is from
the right electrode. This means that there exist only two bands contributing to the electron transmission from the left to the right electrode, which correspond to the eigenchannels $T_1$ and $T_2$ presented in Fig. 8(a). In the second one, from $-0.10$ to $0.15$ eV, there exist four matching bands in the left and right electrodes. These four matching bands, with contribution to the total transmission, correspond to those four conductance channels, especially in which the two degenerate bands $b_1$ and $b_2$ correspond to the degenerate eigenchannels $T_3$ and $T_4$ opening at $-0.1$ eV. There are five matching bands for the left and right electrodes in the third energy region from 0.15 to $-0.20$ eV; specifically, the alignment of band $b_5$ results in the closing of the transmission through the conductance channel $T_1$ at $-0.20$ eV. In the last one, from $-0.20$ to $0.3$ eV, there are four matching bands between the left and right electrodes. In Fig. 10, we display the band matching between the left and right Ag(110) electrodes. Similarly, the bias window in this figure can also be divided into two similar regions as those in the transmission spectra presented in Fig. 8(b). In the first region, from $-0.3$ to $-0.1$ eV, there are three bands in the left electrode, which match the corresponding bands in the right electrode. With the alignment of band $b_1$ at $E=0.05$ eV, leading to the opening of channel $T_4$ shown in Fig. 8(b), there exist four matching bands for the left and right electrodes in the second region from $-0.20$ to $0.3$ eV. In comparison with the Ag(110) electrode, there exist more matching bands in the left and right electrodes, resulting in more channels contributing to the total transmission as well as to the current in the Ag(100) case. In consequence, the application of the bias voltage induces the shift of the electrochemical potential correspondingly, leads to the different band matching of the left and right electrodes, and thus causes different numbers of the eigenchannels contributing to the total transmission and eventually the different currents.

**IV. CONCLUSION**

The electrical transport properties of a Ge$_7$ cluster, which is respectively coupled to two kinds of atomic scale electrodes Ag(100) and Ag(110) with finite cross sections, have been systematically investigated by first-principles calculations. The equilibrium conductance of the Ge$_7$ cluster takes
the value of about 3 and 4 $G_0$ in the case of Ag(110) and Ag(100) electrodes, respectively. Our results clearly show that under strong cluster-electrode coupling, there exists a close correlation between the band structure of the electrode and the transport properties of this cluster under both equilibrium and nonequilibrium conditions. Under zero bias, the number of the electrode bands crossing the Fermi level determines the number of conductance channels of such a cluster and the infinite perfect nanowire consisting of the corresponding electrode. Therefore, for the Ag(100) electrode case, more bands crossing the Fermi level results in a larger conductance than that for the Ag(110) case. By varying the contact distances, our results suggest that for most of investigated distances, the equilibrium conductance of the Ge$_7$ cluster bridging the two Ag(100) electrodes is larger than that in the case of the Ag(110) electrodes. By applying the bias voltages, we find that the nonequilibrium properties of the Ge$_7$ cluster are closely related to the band matching between left and right electrodes for these two cases.

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