

Article

Controllable Synthesis and Characterization of Ordered 0D and 1D Antimony Nanostructures on Ag₂Sb/Ag(111)

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Abstract

By precisely controlling the growth temperature and coverage, we successfully synthesized a highly ordered zero-dimensional (0D) Sb₁₈ nanocluster and a one-dimensional (1D) Janus Sb nanochain on the Ag₂Sb/Ag(111) surface. Using scanning tunneling microscopy (STM) in combination with density functional theory (DFT) calculations, we characterized their atomic structures and found that the alloy substrate plays a significant role in stabilizing these configurations. Our findings not only demonstrate the feasibility of controllably synthesizing low-dimensional Sb nanostructures on metallic substrates but also provide valuable insights into their growth mechanism.

Keywords: nanostructure; scanning tunneling microscopy; density functional theory; antimony

1. Introduction

Antimonene, a two-dimensional (2D) elemental material predicted to possess unique properties including ferroelectricity [1], thermoelectricity [2], and topological characteristics [3], has attracted significant attention in recent years [4]. To date, the two most stable phases of antimonene (α and β phases) have been successfully synthesized on various substrates, including Cu(111) [5], WTe₂ [6] and HfTe₂ [7]. However, studies on other lower-dimensional highly ordered structures of Sb, such as zero-dimensional (0D) nanoclusters and one-dimensional (1D) nanochains or nanoribbons, remain relatively scarce especially from an experimental perspective.

Antimony clusters have attracted considerable interest owing to their near-infrared photothermal properties [8] and their enhanced rate capability and cycling stability as anode materials in rechargeable Li-ion and Na-ion batteries [9]. Despite this interest, their structural understanding remains incomplete. Theoretically, studies have primarily focused on highly ordered nanoclusters smaller than 14 atoms [10–12]. Experimentally, Sb₄ units are the fundamental building blocks during the evaporation process [13,14], and various high-order configurations including trimers, tetramers, and pentamers have been reported on metal surfaces [14,15]. In contrast, larger ordered nanoclusters have received much less attention. Although a theoretical study has predicted that an 18-atom Sb nanocluster



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could significantly enhance the oxygen evolution reaction (OER) [16], such a large, ordered structure has yet to be experimentally observed.

For highly ordered 1D Sb structures, theoretical studies have predicted that their electronic properties can be effectively modulated through stacking or strain engineering [17–19], suggesting significant potential for applications in electronic devices. However, in contrast to these various theoretical works, most experimentally synthesized counterparts reported to date are disordered [15], and their precise atomic structures have yet to be determined.

In this study, the highly ordered 0D Sb nanoclusters and 1D Sb nanochains were fabricated by depositing Sb atoms onto a Ag₂Sb alloy surface above single-crystal Ag(111) under carefully controlled temperatures. Combining scanning tunneling microscopy (STM) and density functional theory (DFT) calculations, we characterized their atomic structures, which were previously unidentified. Our findings demonstrate the feasibility of fabricating ordered low-dimensional Sb nanostructures on metal surfaces and provide deeper insight into the growth mechanisms of Sb on such substrates.

2. Methods

The sample preparation and characterization were performed in an ultrahigh vacuum (UHV) system equipped with connected preparation and STM chambers. The base pressure of the system was maintained below 1×10^{-10} Torr. STM measurements were performed at 5 K with a chemically etched W tip. In this work, the Sb coverage is expressed in monolayers (ML), where 1 ML is defined as the Sb atomic density of a complete Ag₂Sb monolayer, equivalent to an Sb concentration of 4.6×10^{14} atoms/cm².

Our DFT calculations were carried out using the projector-augmented wave method (PAW) [20] as implemented in Vienna ab initio simulation package (VASP, version 6.4.2) [21,22], with the standard PAW pseudopotentials (Sb for Sb and Ag for Ag) employed for all models. The GGA-PBE exchange-correlation functional with a plane-wave cutoff energy of 400 eV was applied to the calculations [23]. The substrate model consisted of a three-layer Ag(111) slab with a single Ag₂Sb surface layer on top, and the bottom atomic layer was kept fixed throughout the relaxation process. An 8×8 alloy supercell and a $2 \times 7\sqrt{3}$ alloy supercell of Ag₂Sb were used to model the 0D nanoclusters and 1D nanochains, respectively. To avoid the spurious interactions along the *c*-direction introduced by the periodical boundary condition, a vacuum layer of 11 Å was included. The Brillouin zone was sampled in $3 \times 1 \times 1$ and $1 \times 1 \times 1$ grids with Γ -point at the center for the 1D and 0D structures, respectively. The energy and force convergence thresholds were set to 10^{-4} eV and 0.01 eV/Å, respectively. As Table S1 in the Supplementary Material shows, convergence tests with respect to both cutoff energy and k-point sampling were performed to ensure that the total energies converged to within 1 meV per atom. All calculations were spin-unpolarized, as the present systems are non-magnetic. Spin-orbit coupling (SOC) and van der Waals (vdW) dispersion corrections were omitted during structural relaxations, as SOC has a negligible impact on atomic geometry and relative formation energy trends, while the binding in the surface alloy/nanostructure is dominated by strong covalent and metallic interactions. The simulated STM images were generated within the Tersoff–Hamann approximation using the P4VASP package. The initial atomic structures were pre-optimized with the Graph-based Pre-trained Transformer Force Field (GPTFF) [24] prior to detailed DFT structure relaxation.

3. Result and Discussion

To obtain high-quality Ag₂Sb alloy substrates for subsequent experiments, a single-crystal Ag(111) surface was first cleaned by standard Ar⁺ ion sputtering and annealing cycles. Then the Sb₄ clusters were evaporated from a Knudsen cell and deposited onto this surface, replacing the surface Ag atoms and ultimately forming the Ag₂Sb alloy layer [5,25]. During

this process, the Knudsen cell source was maintained at approximately 500 K, with an Sb flux of about 0.2 ML/min. Prior to Sb deposition, both the Knudsen cell and the Ag(111) substrate were preheated at the target temperature for 10 min to ensure thermal equilibration.

According to previous reports, further deposition of Sb₄ clusters onto the Ag₂Sb surface at 360 K can subsequently lead to the formation of α -antimonene [5]. In contrast, deposition at room temperature may cause the surface to become predominantly covered by irregular Ag₂Sb alloy islands and dispersed Sb clusters, as shown in Figure S1. However, as shown in Figure 1a, we observed that when approximately 2.2 ML of Sb atoms were deposited on the Ag(111) surface at a lower temperature of about 330 K, the surface became covered with one-dimensional (1D) Sb nanochains. Interestingly, these narrow nanochains exhibit a highly ordered orientation, as illustrated in Figure 1b. The bright protrusions observed on the substrate correspond to Sb atoms incorporated into the Ag₂Sb alloy, whose periodicity matches $\sqrt{3}$ times the lattice constant of Ag, indicating that one-third of the Ag atoms in the topmost layer are substituted by Sb atoms [5,25]. Based on the STM analysis, these nanochains align with the high-symmetry directions of the Ag₂Sb surface alloy and the $[11\bar{2}]$ direction of the Ag(111) substrate.

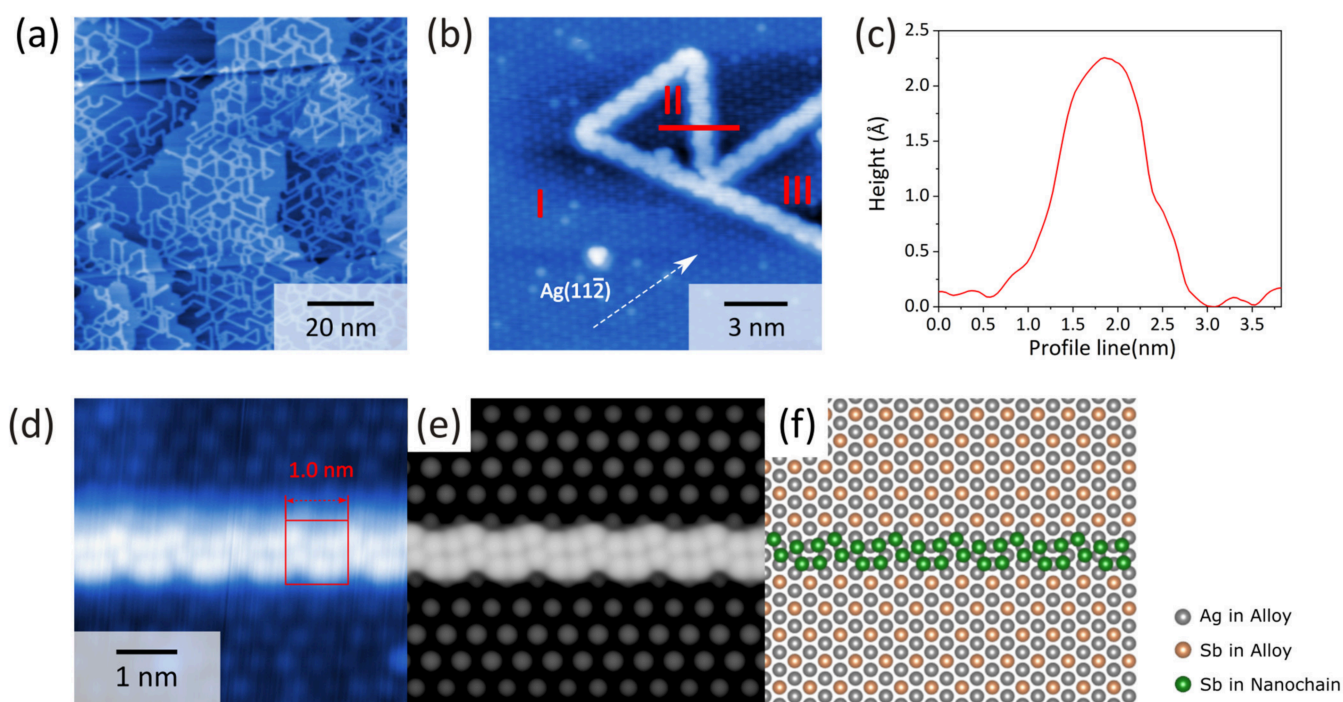


Figure 1. (a) Large-scale STM image ($V_{\text{tip}} = -0.96$ V, $I_{\text{tip}} = -30$ pA) of the surface topography with a 2.2 ML Sb coverage on the Ag(111) surface. (b) The STM image (-1.2 V, -100 pA) of the 1D Sb nanochains. The dashed white arrow indicates the high-symmetry directions of the Ag₂Sb surface alloy. The labels I, II, and III indicate different alloy substrate regions. (c) Height profile from (b). (d) High-resolution STM image (-0.1 V, -150 pA) of the 1D Janus Sb nanochain. (e) Simulated STM topographic image of (f), using an energy window of 0–0.1 eV above the Fermi level. (f) Atomic structure model of 1D Janus Sb nanochain.

Furthermore, we found that the Ag₂Sb alloy regions (labeled as I, II, and III in Figure 1b) on either side of the nanochains exhibit a noticeable lattice mismatch in the STM images, which indicates that these nanochains reside at the domain boundary between two distinct alloy regions and thus function as a structural “domain wall” [26]. Meanwhile, as shown in Figure 1c, these nanochain walls exhibit a height of approximately 0.22 nm above the substrate, which closely matches the characteristic height of a single atomic layer.

A previous study by Sun et al. [15] reported similar nanochains composed of discrete small clusters. In contrast, our high-resolution STM image shown in Figure 1d suggests that the present nanochains exhibit a highly ordered zigzag structure consisting of six-atom repeating units. It is worth noting that this configuration presents a distinct Janus characteristic which features an asymmetric structure along its axis, setting it apart from conventional nanochain structures reported previously. The term “Janus” here denotes structural asymmetry specific to the Sb nanochains and is distinct from its usage in the graphene-based system [27]. Furthermore, the measured periodicity of these Janus nanochains is approximately 1 nm, equivalent to twice the lattice constant of the Ag₂Sb substrate.

DFT calculations have proven effective in exploring the structural stability and electronic properties of nanostructures [28,29]. To clarify the structure of these 1D Janus nanochains which reside at the alloy boundary, we constructed their atomic model which is shown in Figure 1f according to the experimental STM image. As shown in Figure 1d,e, the simulated STM image based on the proposed structure is in good agreement with the experimental STM image, which is consistent with the proposed Janus atomic structure.

To elucidate the formation mechanism of the Janus structure, we considered two additional models: (I) a nanochain on a Ag₂Sb substrate without a domain boundary, and (II) a model based on Figure 1f but with a higher Sb atom density at the domain boundary. Their simulated STM images are shown in Figure S2a,b in the Supplementary Materials, respectively. The former is not consistent with the experimental result, while the latter shows no significant difference from Figure 1e. Given that STM image contrast alone does not allow us to distinguish between these models, we computed the formation energies of nanochains on Ag₂Sb substrates of all three models shown in Figure 2a–c, respectively, as summarized in Table 1. Here the formation energies of the nanostructures were calculated using the following expression:

$$E_{\text{formation}} = E_{\text{total}} - E_{\text{sub}} - \sum n_i \mu_i \quad (1)$$

where μ_i represents the chemical potential of single Sb or Ag atom in its bulk phase, n_i represents the related number of atoms in the nanostructure, E_{total} represents the energy of the nanochain with the substrate, and E_{sub} represents the energy of the substrate.

Table 1. The formation energies of the structural models presented in Figure 2. All models are based on a $2 \times 7\sqrt{3}$ alloy supercell of Ag₂Sb.

Model	Composition	E_{sub}	$E_{\text{formation}}$ (eV)
Domain boundary (2a)	6 Sb	−934.47	−1.84
No boundary (2b)	6 Sb	−941.80	1.49
High Sb density at boundary (2c)	6 Sb	−938.48	0.85
Ag-substituted site 1 (2d)	5 Sb + 1 Ag	−934.47	−1.14
Ag-substituted site 2 (2e)	5 Sb + 1 Ag	−934.47	−1.01

As shown in Table 1, our results clearly demonstrate that Janus nanochains positioned along alloy boundaries with a high Sb density exhibit lower formation energies than those on continuous alloy regions or those with a higher Sb density at the boundaries, supporting the assignment that low-density domain boundaries play a crucial role in stabilizing the Janus configuration. Our findings not only indicate a strong interaction between the Sb atoms and the underlying Ag₂Sb alloy substrate, but also offer deeper insight into the atomistic self-assembly processes of Sb on metal surfaces.

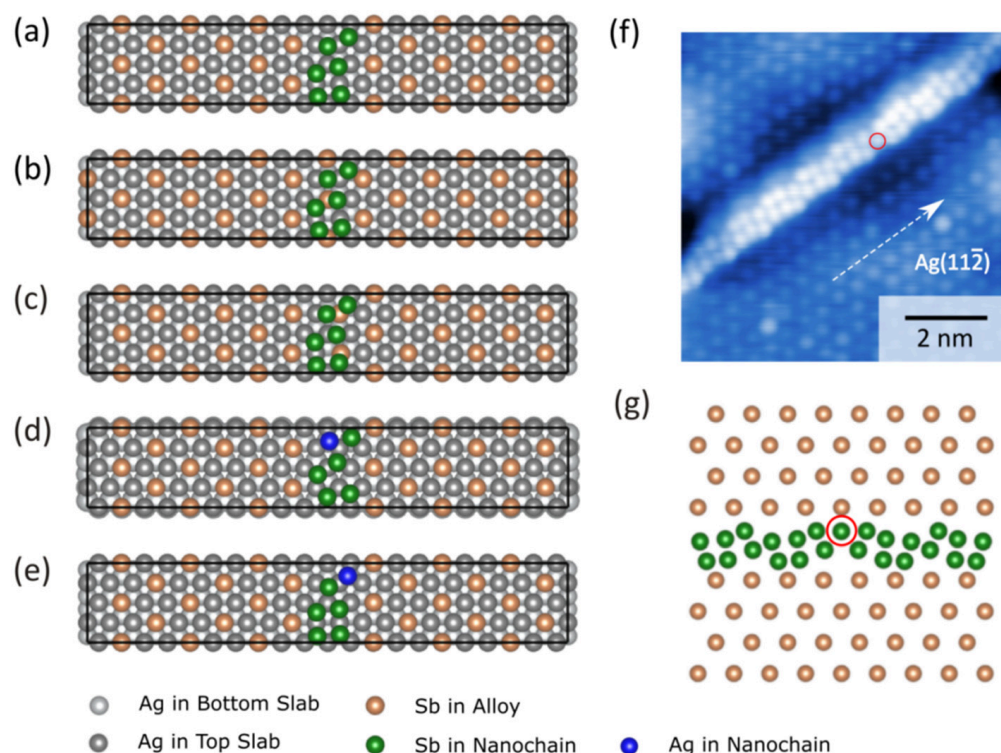


Figure 2. Atomic structure model of 1D Janus Sb nanochain on Ag_2Sb substrates. The black rectangle indicates the unit cell used in our calculations. (a) Sb nanochain on the Ag_2Sb substrate with a domain boundary. (b) Sb nanochain on the Ag_2Sb substrate without a domain boundary. (c) Model based on (a) but with a higher Sb atom density in the substrate. (d,e) Two models based on (a) but with mixed Ag-Sb compositions. (f) High-resolution STM image (-0.1 V, -100 pA) of an Sb nanochain composed of two structural components with opposite symmetry. The red circle highlights a bright Sb atom that bridges the two nanochains. The dashed white arrow indicates the high-symmetry directions of the Ag_2Sb surface alloy. (g) Atomic structure model corresponding to the configuration shown in (f). The red circle in (g) corresponds to the red circle in (f).

Meanwhile, as shown in Figure 2d,e, to verify whether the nanochains consist solely of Sb atoms, we substituted selected Sb sites with a Ag atom within the nanochain structure and computed their corresponding system energies. As shown in Table 1, our calculations clearly demonstrate that the incorporation of Ag atoms significantly increases the formation energy of the systems. Meanwhile, as their simulated STM images (Figure S2c,d in Supplementary Materials) show, the Ag atoms in the nanochain appear darker than the Sb atoms in the simulated STM images, which is inconsistent with our experimental results. Both findings support the assignment that a pure Sb composition represents the most stable configuration for the observed nanochains.

Furthermore, we observed that two nanochains sharing the same orientation but exhibiting opposite symmetry can join to form an integrated structure, as seen by the high-resolution STM image in Figure 2f. These nanochains are connected via a single Sb atom which is marked with a red circle. The corresponding schematic atomic model in Figure 2g clearly illustrates this bridging configuration, in which a single Sb atom links the two nanochains at their junction. This distinctive connection mode not only preserves the Janus feature of each individual nanochain but also results in a stable and continuous superstructure. Such a bridging mechanism underscores the flexibility and adaptability of Janus Sb nanochains in self-assembling into complex architectures on the Ag_2Sb surface.

When the Sb coverage was reduced to 1.4 at the same substrate temperature, in addition to the ordered Janus 1D nanostructures, we observed another type of disordered nanochain which consists of various self-assembly clusters on the Ag_2Sb surface, as shown

in Figure 3a. Among these features, small clusters such as trimers, tetramers, and pentamers were identified, consistent with previous reports by Sun [15]. Notably, we discovered a new type of nanocluster (marked by red squares) with a volume several times greater than those previously observed. A high-resolution STM image of an individual larger nanocluster in Figure 3b suggests a highly ordered six-fold symmetric structure, consisting of an inner and an outer ring. The inner ring adopts a benzene-like hexagonal arrangement, while the outer ring is composed of six Sb dimers. Meanwhile, as illustrated in Figure 3c, the inner ring appears slightly higher than the outer one in STM topography. This special configuration suggests a nanocluster comprising 18 Sb atoms, representing a structure notably larger than any previously reported Sb nanoclusters in this system. Remarkably, despite its substantial size, the nanocluster maintains a highly symmetric and stable morphology, making it of considerable scientific interest.

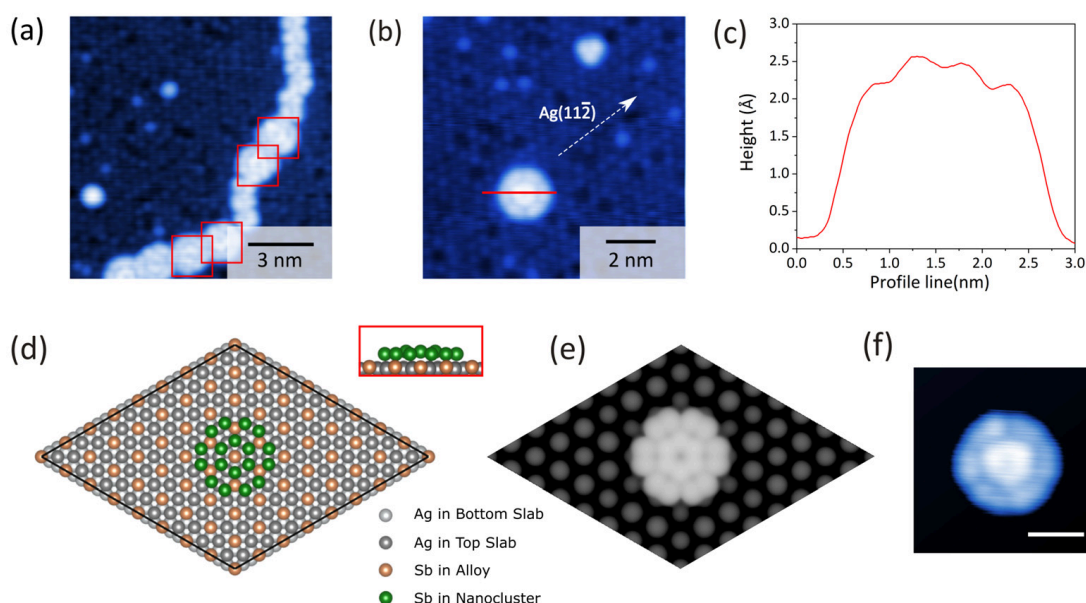


Figure 3. (a) STM image (-0.1 V, -150 pA) of a disordered 1D Sb nanochain formed by various clusters. The red frame marks a previously unreported large nanocluster. (b) STM image (-0.2 V, -100 pA) of an individual large Sb nanocluster. The dashed white arrow indicates the high-symmetry directions of the Ag_2Sb surface alloy. (c) Height profile from (b), indicating topographic variation across the nanocluster. (d) Atomic structure model of the Sb_{18} cluster with a side-on perspective shown in the inset. (e) Simulated STM topographic image of (d), using an energy window of 0 – 0.2 eV above the Fermi level. (f) High-resolution STM image (-0.2 V, -100 pA) of the Sb_{18} cluster. The white scale bar represents 1 nm, and the image is displayed at the same scale as in (e).

To elucidate the atomic structure of the large nanocluster, we constructed a corresponding structural model based on the experimental data, as shown in Figure 3d. Upon structural relaxation, the model predicts that the atoms in the inner ring are positioned slightly higher than those in the outer ring, which is also consistent with the experimental observations, thereby further supporting the proposed model and suggesting a strong interaction from the underlying substrate. Furthermore, as shown in Figure 3e, the simulated STM image derived from this model is also compatible with the experimental STM image in Figure 3f, in terms of both morphology and dimensions. This proposed model indicates the existence of a previously unreported, highly symmetric Sb_{18} nanocluster. Its emergence markedly enriches the structural diversity within the antimony cluster family. Furthermore, it demonstrates that complex and ordered Sb architectures can be synthesized controllably on the Ag_2Sb alloy surface, providing a new paradigm for the design of low-dimensional nanostructures.

4. Conclusions

In summary, we have successfully synthesized two new types of highly ordered low-dimensional Sb nanostructures: a 1D nanochain and a 0D nanocluster on a Ag₂Sb/Ag(111) surface. By combining STM and DFT calculations, we characterized their atomic configurations: the 1D Sb nanochain consists of six-atom repeating units and exhibits a unique Janus zigzag structure, whereas the 0D Sb nanocluster comprises 18 atoms and displays a distinct six-fold symmetry. Our work not only demonstrates the feasibility of constructing highly ordered low-dimensional Sb nanostructures on metal surfaces, but also provides a deeper understanding into their growth mechanism.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/cryst16090583/s1>, Figure S1: STM image of 1.4 ML Sb atoms deposited on Ag(111) at room temperature; Figure S2: Simulated STM topographic images corresponding to Figure 2b–e, respectively, using an energy window of 0–0.1 eV above the Fermi level; Table S1: Calculated energies of the same model under different computational conditions.

Author Contributions: Conceptualization, P.Z.; software, J.C.; validation, P.Z. and J.T.; formal analysis, J.C.; investigation, P.Z., H.L. and C.M.; resources, Y.L. (Yun Li) and L.C.; data curation, P.Z., J.T., X.W. (Xiaohuai Wang) and X.W. (Xiang Wang); writing—original draft preparation, P.Z.; writing—review and editing, S.S., Y.L. (Yun Li) and Y.L. (Youming Lu); visualization, J.T.; supervision, Y.L. (Yun Li); project administration, P.Z.; funding acquisition, P.Z. and Y.L. (Yun Li). All authors have read and agreed to the published version of the manuscript.

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Data Availability Statement: The data presented in this study are available on request from the corresponding author.

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