

## Electronic Supplementary Information for “La induced Si<sub>3</sub> trimer bilayer on Si(111) surface”

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**(1) The atomic structures of the different La coverages induced Si(111) surface reconstructions.**

Figure S1 shows the different La coverages induced Si(111) surface reconstructions. For  $(3 \times 2)$ ,  $(5 \times 2)$ ,  $(7 \times 6)$  and  $(2 \times 3)$  reconstructions [Fig. 1(a-d)], their surface layer are consisted of Si chains along  $y[\bar{1}10]$  direction separated by channels that accommodate La atoms. The  $(3 \times 2)$  reconstruction [see Fig. S1(a)]<sup>1</sup> is only formed by honeycomb chains with the La coverage of  $1/6$  ML [one La atom per surface unit cell], where La atoms are located on the top site  $T_4$  of Si(111) surface in the channel. The  $(5 \times 2)$  reconstruction [see Fig. S1(b)]<sup>2,3</sup> is formed by a combination of alternatively arranged honeycomb and Seiwatz chains with the La coverage of  $1/5$  ML, where two La atoms per surface unit cell are located at hollow site  $H_3$  and top site  $T_4$  of Si(111) surface in two neighboring channels, respectively. The  $(7 \times 6)$  reconstruction [see Fig. S1(c)]<sup>4</sup> consists of one honeycomb and two Seiwatz chains with the La coverage of  $10/42$  ML, where ten La atoms per surface unit cell (five La atoms at  $H_3$  site and five at  $T_4$  site) are distributed as evenly as possible in three neighboring channels. The  $(2 \times 3)$  reconstruction [see Fig. S1(d)]<sup>4,5</sup> is only constructed by pure Seiwatz chain, which contains one La atom per surface unit cell that located at  $T_4$  site, corresponding to  $1/3$  ML. For the  $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$  reconstruction<sup>2</sup> in see Figure S1(e), its each surface unit cell contains six La atoms forming a hexagonal structure, which are adsorbed on  $T_4$  site, in this way requiring a La coverage of  $1/2$  ML.

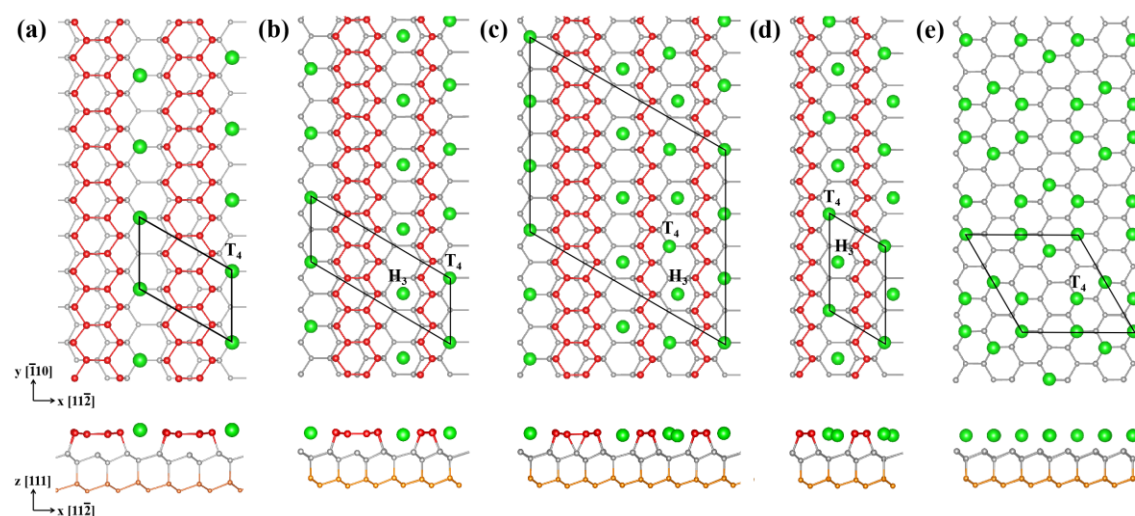


Fig. S1: Top view (upper panel) and side view (lower panel) of the possible reconstructions induced by different coverage La atoms on Si(111) surface. (a) The  $(3 \times 2)$  HCC reconstruction with La coverage of  $1/6$  ML; (b) The  $(5 \times 2)$  HCC+SC reconstruction with La coverage of  $1/5$  ML; (c) The  $(7 \times 6)$  HCC+SC reconstruction with La coverage of  $10/42$  ML; (d) The  $(2 \times 3)$  SC reconstruction with La coverage of  $1/3$  ML; (e) The  $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$  reconstruction with La coverage of  $1/2$  ML. The surface unit cell of these structures are mapped by solid lines. The red spheres represent surface Si layer, the gray spheres represent first Si layer of Si(111) surface, and orange spheres represent the deeper Si layer. Green spheres represent La atoms.

## (2) The experimental STM images of La/Si(111)- $(\sqrt{3} \times \sqrt{3})R30^\circ$ reconstruction.

Figure S2 shows the experimental STM images of La/Si(111)- $(\sqrt{3} \times \sqrt{3})R30^\circ$  reconstruction reported by Liu *et al.*<sup>6</sup>

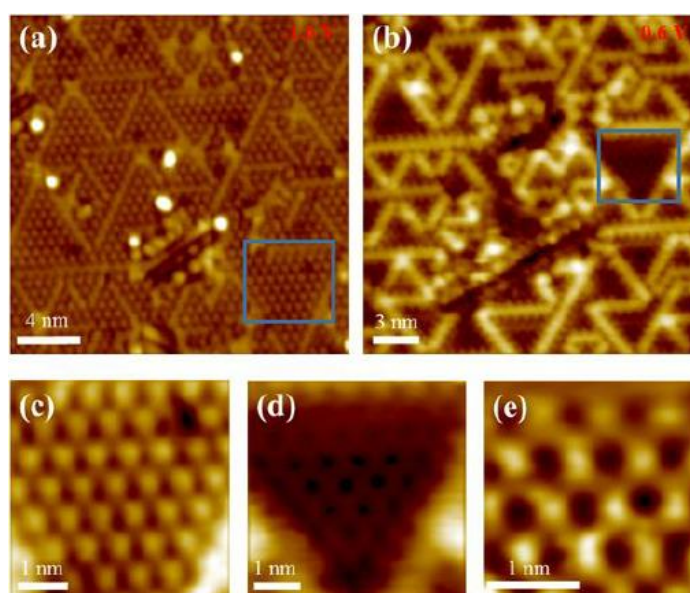


Fig. S2 The experimental STM images of La/Si(111)- $(\sqrt{3} \times \sqrt{3})R30^\circ$  reconstruction at (a) negative voltage bias (-1.6 V) and (b) positive voltage bias (0.6 V). (c) The zoomed-in picture of the blue box area in (a). (d) The zoomed-in picture of the blue box area in (b). (e) The zoomed-in morphology of the interior surrounded by triangle boundaries in (d).<sup>6</sup>

## References

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