Supplemental Information

Robust Atomic-Structure of the 6×2 Reconstruction Surface of Ge (110) Protected by the Electronically Transparent Graphene Monolayer

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Our DFT calculations were performed by using the Vienna *ab initio* simulation package [1]. The generalized gradient approximation (GGA) function in the Perdew–Burke–Ernzerh form was used to describe the exchange correlation interactions [2]. The projector augmented wave potential [3] was employed to describe the electron–ion interaction. The cut-off energy for the plane–wave expansion is set to 400 eV. A Fermi-broadening of 0.2 eV [4] was chosen to smear the occupation of the bands around the Fermi energy by using a finite-T Fermi function and by extrapolating to T = 0 K. The calculated lattice constant for bulk Ge was 5.783 Å, slightly larger than the experimental value of 5.66 Å. This overestimation is common for GGA calculations due to its underestimation on chemical bonding strengths.

The Ge (110) surface was modeled using a slab of five Ge atomic layers and an additional adatom layer to form reconstruction patterns. The dangling bonds of the

bottom Ge layer were saturated with H atoms. A 20 Å vacuum layer was used to separate neighboring Ge slabs. The in-plane supercell size was set to be (6 × 2) following the experimental findings. Note that the supercell size was 21.25 Å × 14.16 Å in theoretical calculations, slightly different from the experimental values of 20.8 Å × 13.9 Å, because we adopted the relaxed lattice constant of 5.783 Å instead of the experimental value. Because of the relatively small Brillouin Zone for the (6 × 2) supercell, and limited computing abilities, we used a single Gamma point to represent for the Brillouin Zone. During geometric optimizations, the bottom layer of Ge atoms was fixed, while all other Ge and H atoms were free to relax until the forces on them were smaller than 0.01 eV/Å along each direction. The lattices of the supercell were fixed among geometry optimizations.

The STM simulation was carried out following the theory presented by Tersoff and Hamann [5]. In this theory, the tunneling current was proportional to the local density of states of the surface, at the position of the tip.

[1] Kresse G.; Hafner J. Ab initio molecular dynamics for liquid metals. Phys. Rev. B 1993, 47, 558, and references therein.

[2] Perdew J. P.; Burke K.; Ernzerhof M. Generalized Gradient Approximation Made Simple. Phys. Rev. Lett. 1996, 77, 3865.

[3] Blöchl P. E. Projector augmented-wave method. Phys. Rev. B 1994, 50, 17953.

[4] Weinert M.; Davenport J.W. Fractional occupations and density-functional energies and forces. Phys. Rev. B 1992, 45, 13709.

[5] Tersoff J.; Hamann D. R. Theory of the scanning tunneling microscope. Phys. Rev. B 1985, 31, 805-813.Kresse G.; Hafner J., *Phys. Rev. B* **1993**, 47, 558, and references therein.

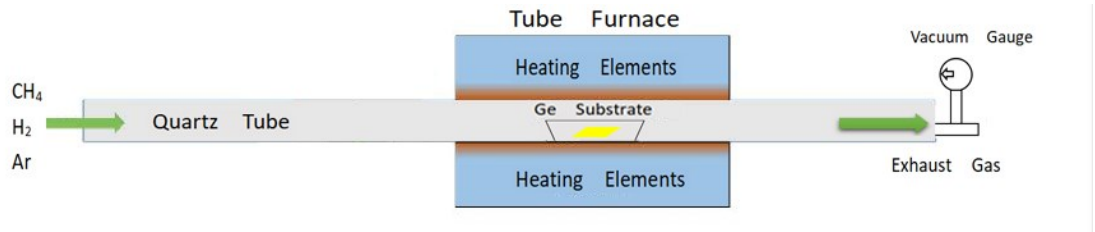

Figure S1 The CVD setup for growing the graphene monolayer on Ge(110) substrate surface

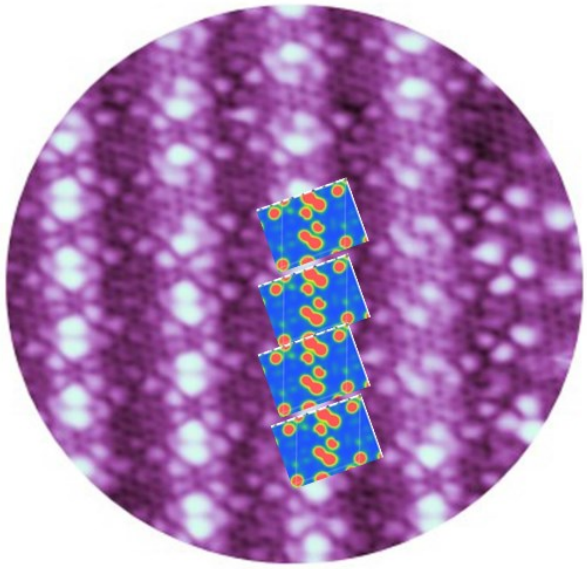

Figure S2 A representative high-resolution STM image superimposed the ball-and-stick model of Ge(110)-6 ×2 reconstruction calculated by DFT. It clearly shows a good consistence between the ball-and-stick model and the real STM image.

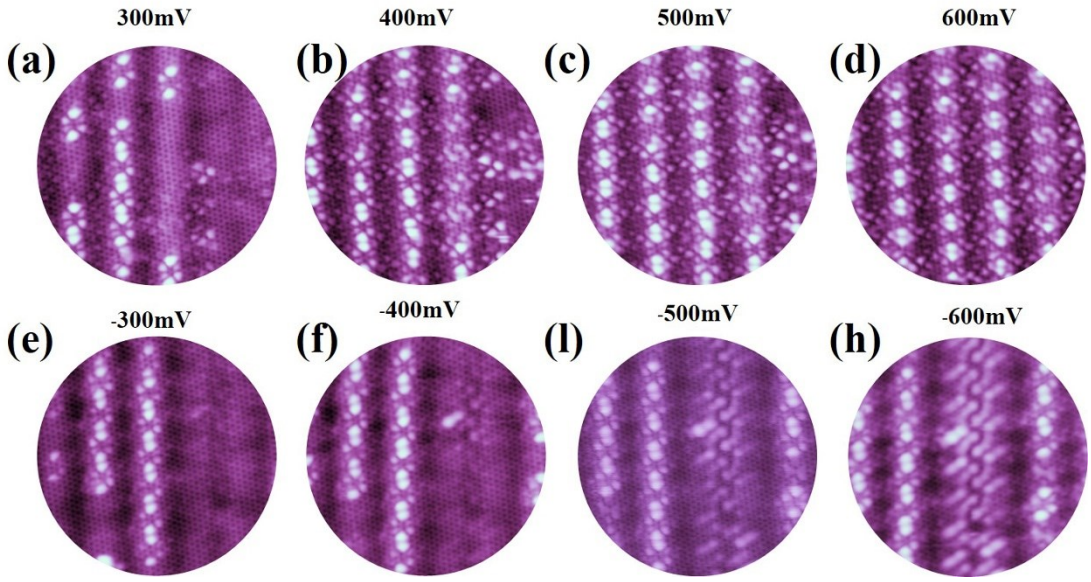

Figure S3 (a-h) The high-resolution STM images scanned under the different tip biases, which clearly show that the topographic structure of Ge(110)-6×2 reconstruction surface is robust and can be selectively resolved with the scanning bias beyond 500 mV. However, for the case of the negative sample biases, the STM images shows a honeycomb feature, which exhibits the graphene structural characteristics. Moreover, a series of STM images from e to h show the square wave function shape structure. We deduce that this peculiar structure might be the grain boundary according to the observation of the anti-parallel packing adatoms.