Supporting Information:

Membrane Destruction and Phospholipids Extraction by Two Dimensional MoS_2 nanosheets

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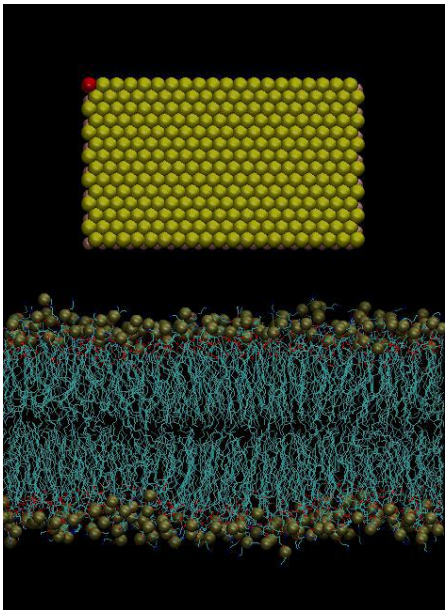

Fig. S1 The initial structure of the released simulation system. The free MoS_2 nanosheet was put above the membrane vertically. In the z direction, the COM distance between the MoS_2 nanosheet and the lipid membrane was 1.97 nm. The restricted S atom at the start of simulation denoted in red.

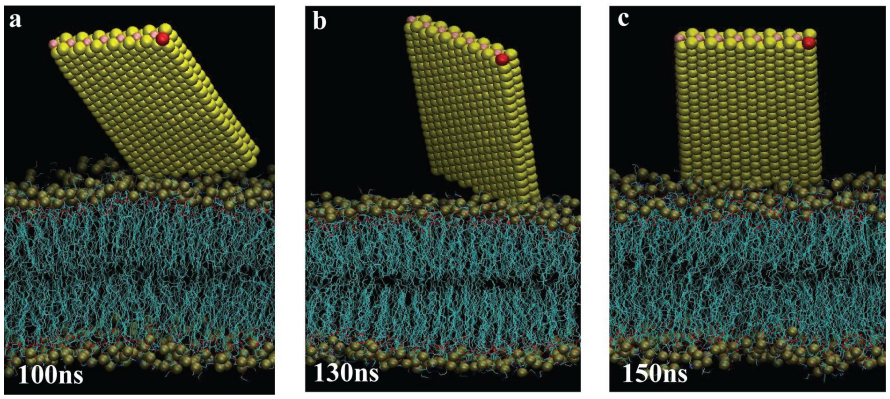

Fig. S2 The profile of the restrictive simulation at specific time between t= 77 ns - 169 ns. As can be seen, the lower left (Fig. S2a) or right (Fig. S2b) corner of MoS_2 nanosheet was in contact with the lipid membrane at t= 100 ns and t= 130 ns. At t= 150 ns, the whole unfixed bottom edge of MoS_2 nanosheet contacted the cell membrane.

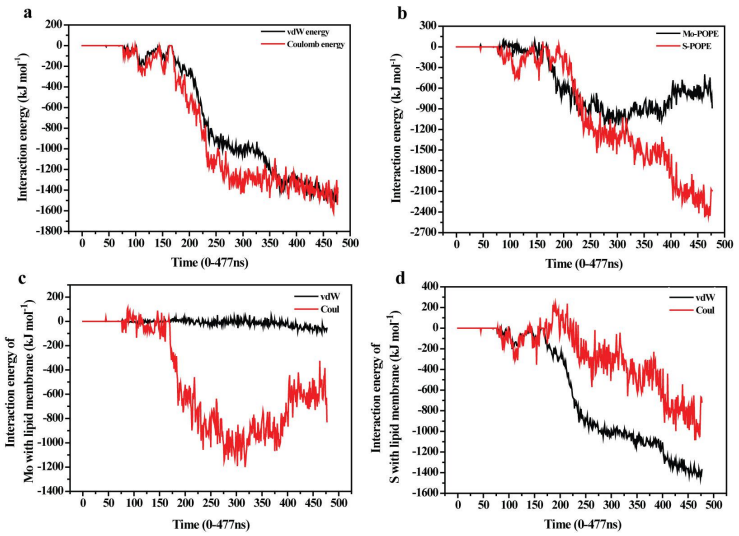

Fig. S3 The interaction energy during the restrictive simulation. (a) the van der Waals (black) and Coulomb (red) energies between MoS_2 nanosheet and lipid membrane. (b) the interaction energies of Mo (black) and S (red) with lipid membrane. (c-d) the van der Waals (black) and Coulomb (red) energies of Mo and S with lipid membrane.

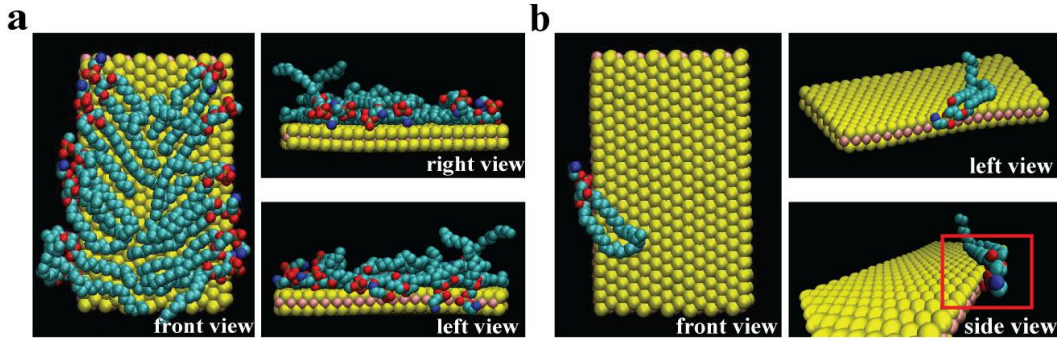

Fig. S4 (a) the images of the extracted phospholipid molecules that adhered on the MoS_2 surface at t= 477 ns in the restrictive simulation. (b) the images of a simple extracted lipid molecule that attracted to the lateral edge of MoS_2, the side view amplifies the attached image of the lipid head group (as indicated by the red box). Colour settings are as in Fig. 1.

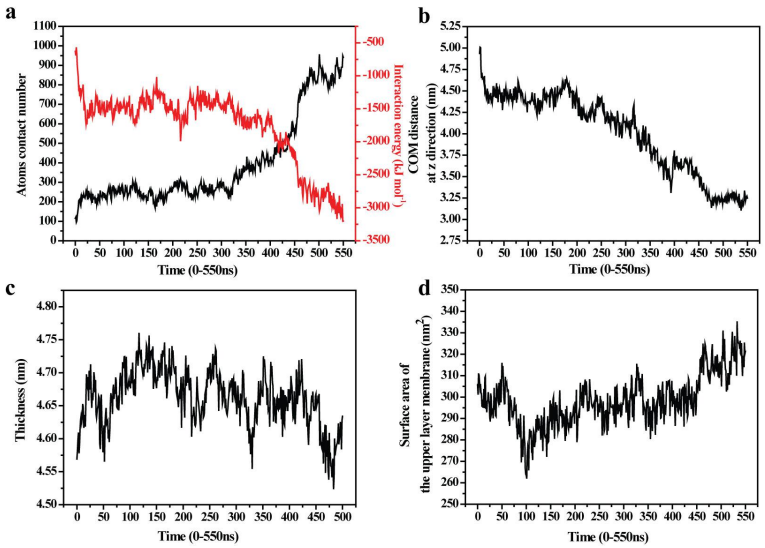

Fig. S5 Released simulation process. (a) the interaction energy and atom contact number between MoS_2 nanosheet and membrane. (b) the centre of mass (COM) distance between the MoS_2 nanosheet and lipid membrane in z direction. (c) the thickness of membrane. (d) The surface area of the upper layer.

As shown in Figs. S5c-d, the change of membrane thickness is similar to the restrictive simulation. At t= 306 ns - 460 ns, the membrane thickness slightly decreased because of the embedding of MoS_2 nanosheet. And after t= 460 ns it began to increase, corresponding to the membrane expansion during the extraction stage. As for the surface area of the upper layer, in the early stage it steadily decreased under the interference of MoS_2 nanosheet. After t= 306 ns, the extraction of lipid molecule increased the surface area. Taken together the behavior of surface area of upper layer in released simulation is similar to that of the restrictive simulation.

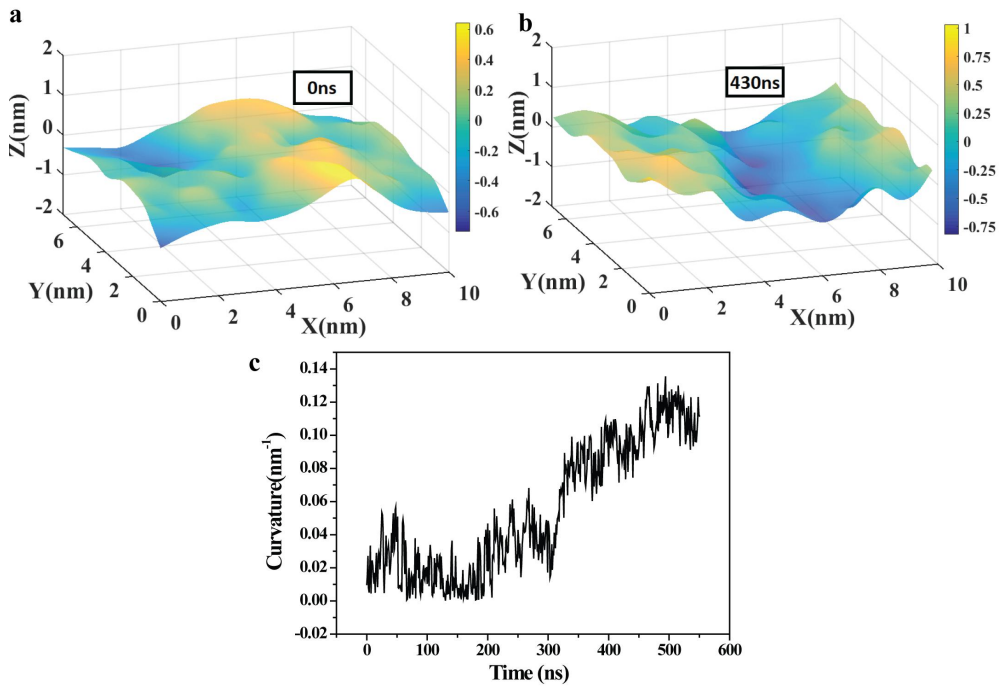

Fig. S6 Analyses of the dent on the surface of lipid membrane during the released simulation. (a) the morphology of the upper layer at the start of simulation. (b) the morphology of the upper layer at t= 430 ns. The average z coordinate value of the entire surface was set to 0. (c) curvature of the upper layer as a function of time in the released simulation.

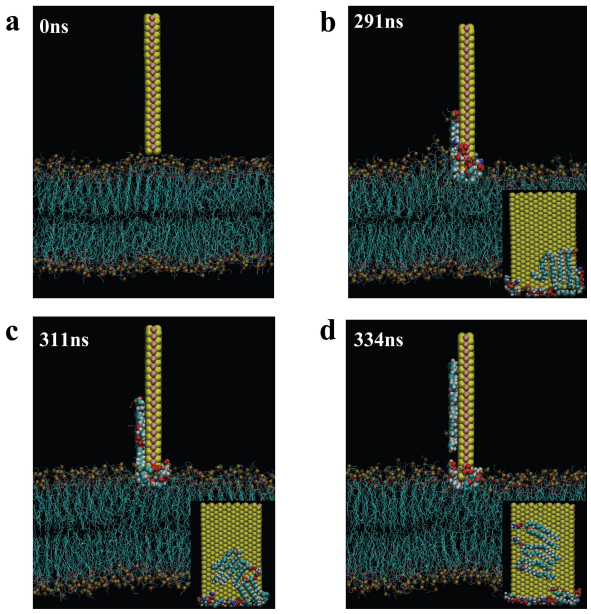

Fig. S7 Representative trajectories of the docking simulation. (a-d) snap-shots of the simulation at 0, 291, 311, and 334 ns, respectively. Colour settings are as in Fig. 1, and with water hidden for clarity here. The illustrations exhibit the images of the extracted phospholipid atoms within 5 Å of MoS_2 nanosheet.

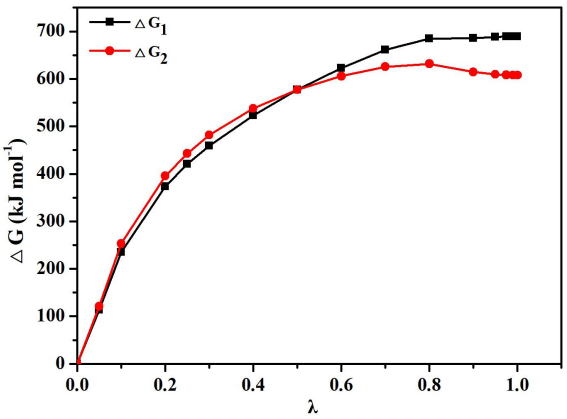

Fig. S8 The cumulative free energy differences ΔG (λ) (=G(λ)-G(0)), averaged over 5 independent simulations, for annihilating a lipid in the membrane (ΔG_2), on the MoS_2 surface (ΔG_1).

ΔG can be obtained from the following ensemble average,

$$\Delta G = -k_B T \ln < (V_f - V_i)/k_B T >,$$

where k_B is the Boltzmann constant; T is the temperature; V_i and V_f are interaction energies at the initial (i) and the final (f) stages. Here, V contains both dispersive and electrostatic interaction. To be accurate, multiple intermediated stages (denoted by λ) are inserted, yielding a gradual annihilation process. λ= 0 and 1 correspond to the initial (with a lipid equilibrated on its substrate) and the final (with a lipid annihilated on its substrate) states, respectively.

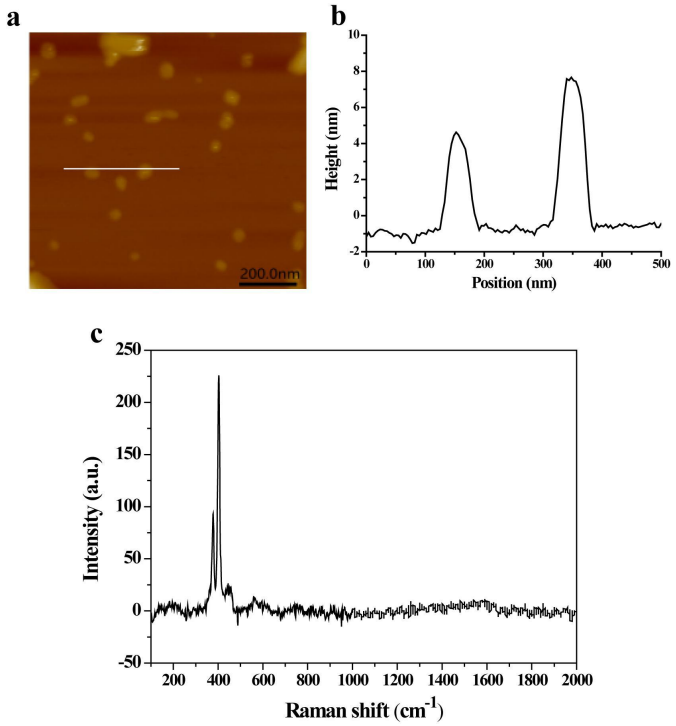

Fig. S9 AFM characterization and Raman spectra of MoS_2 nanosheets. The cross-sectional profile of these two MoS_2 nanosheets (a) suggest that the thickness of the MoS_2 nanosheet was about 4.48 nm and the size of MoS_2 nanosheet was about 100 nm. (b) Two distinct peaks of 377.6 (cm^{-1}) and 402.7 (cm^{-1}) of MoS_2 nanosheets in the Raman spectra consistent with previous studies. They are corresponding to the two vibrational modes of E_{2g}^1 and A_{1g} of MoS_2 respectively.

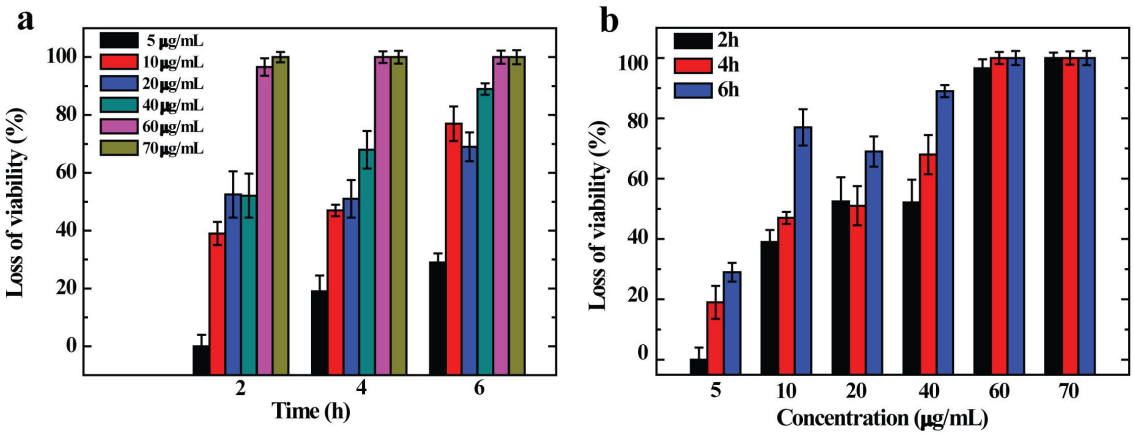

Fig. S10 Antibacterial activity of MoS_2 nanosheets towards *E. coli* DH5α. (a) time dependent loss of vability of *E. coli* under disposing with different concentration of MoS_2 nanosheets, (b) concentration dependent loss of vability of *E. coli* incubated with different dispersions of MoS_2 nanosheets for 2, 4, 6 h.

As can be seen, the antimicrobial properties of MoS_2 nanosheet increased with time and concentration. As shown in Fig. S10a, when the incubation time prolonged from 2 h to 4 h, the antibacterial effect was almost achieved at one hundred percent. And the loss of viability of *E. coli* DH5α treated by MoS_2 nanosheets at 60 μg mL^{-1} for 2 h was more than twice times of which exposed to 10 μg mL^{-1} that would arrived at 39%.

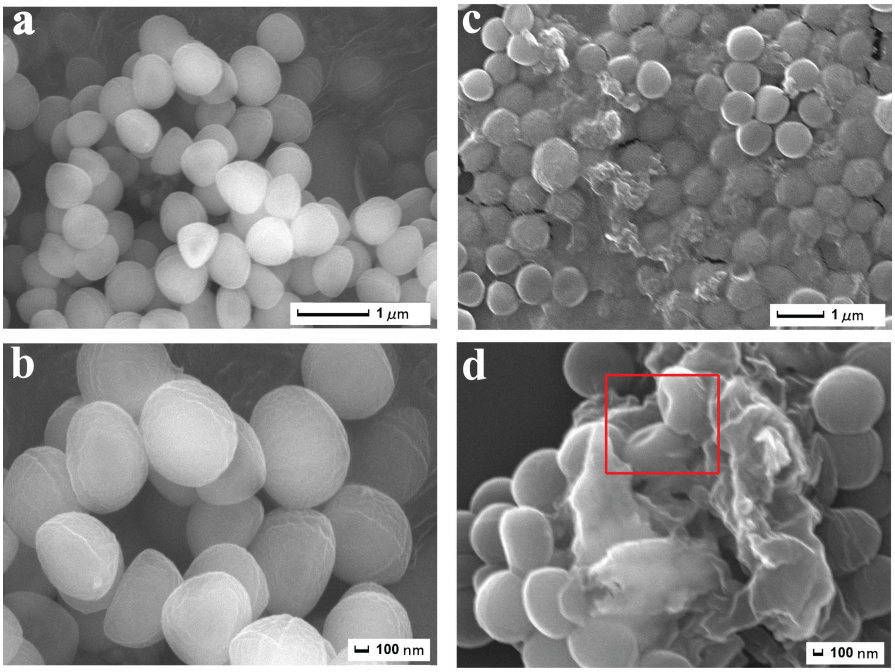

Fig. S11 SEM images of *S. aureus* alone and the one treated by MoS_2 nanosheets. (a-b) the *S. aureus* in the control group. (c) the *S. aureus* with the incubation of MoS_2 nanosheets on the concentration of 40 μg mL^{-1} at 37 ℃ for 4 h. (d) the dent area on the surface of *S. aureus* treated by MoS_2 nanosheets (red squareness).

To explore the effect of MoS_2 nanosheets on *S. aureus*, the morphologies of *S. aureus* with and without the treatment of MoS_2 nanosheets were studied by using SEM. The *S. aureus* in the control group showed intact cell morphology (Figs. S11a-b), but the one treated by MoS_2 nanosheets became flattened and wrinkled (Fig. S11c). The loss of viability and the damage to the cell membrane could be found. In addition, we also observed the dent on the cells treated by MoS_2 nanosheets (Fig. S11d). It is also consistent with the results we obtained in molecular dynamic simulations.

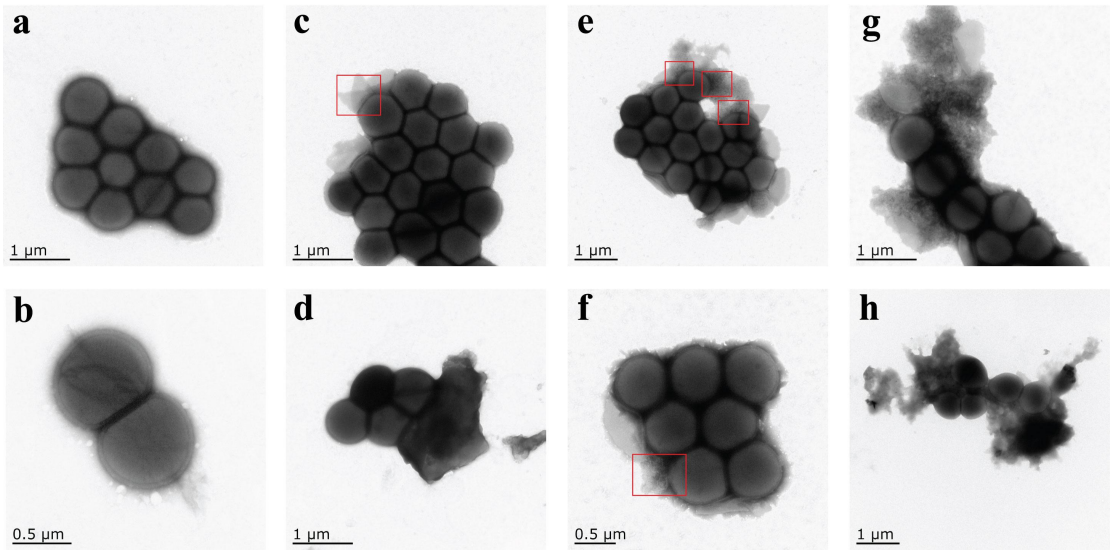

Fig. S12 TEM images of *S. aureus* alone and the one treated by MoS_2 nanosheets with the concentration of 40 μg mL^{-1}. (a-b) the *S. aureus* in the control group. (c-d) the *S. aureus* contacting with MoS_2 nanosheets. (e-f) the damaged *S. aureus* with some loss of cytoplasm. (g-h) the ultimately damaged *S. aureus*.

To further verify the destructive effect of MoS_2 on the membrane of *S. aureus*, Fig. S12 presented the TEM images of *S. aureus* with and without the treatment of MoS_2 nanosheets. As can be seen in Figs. S12a-b, the cell walls and membranes of *S. aureus* in the control group were intact and smooth. However, after treating by MoS_2 nanosheets, the cell membranes of *S. aureus* became rough and even disappeared. Figs. S12c-d showed the direct evidence of the interaction of bacteria with MoS_2 nanosheets. As the interaction intensified, *S. aureus* began to break down and the cytoplasm flowed out (Figs. S12e-f). There were more cytoplasm released (Figs. S12g-h), which eventually resulted in the death of *S. aureus*.

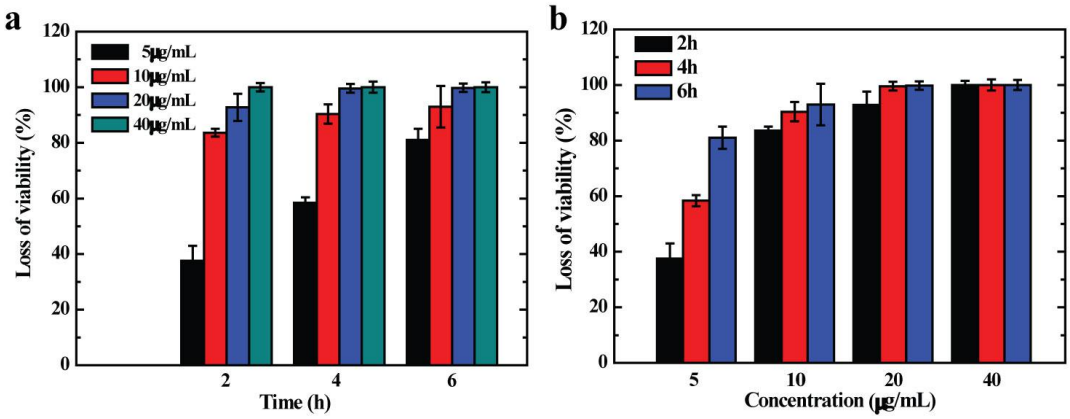

Fig. S13 Antibacterial activity of MoS_2 nanosheets against *S. aureus*. (a) the loss of viability of *S. aureus* with the treatment of MoS_2 nanosheets on different concentrations vs. time, (b) concentration dependent loss of vability of *S. aureu*s incubated with MoS_2 nanosheets for 2, 4, 6 h, respectively.

Similar to *E. coli*, the antibacterial properties of MoS_2 nanosheets against *S. aureus* increased with time and concentration. Compared to *E. coli*, *S. aureus* is more likely to be killed by MoS_2 nanosheet. MoS_2 nanosheets with the concentration of 20 μg mL^{-1}, can completely kill the *S. aureus* after 4 h incubation.