# Supplementary Information

## Regulation of Protein Translocation through A $Si_3N_4$-CNT Stacked Nanopore Using An Embedded Gold Nanoparticle

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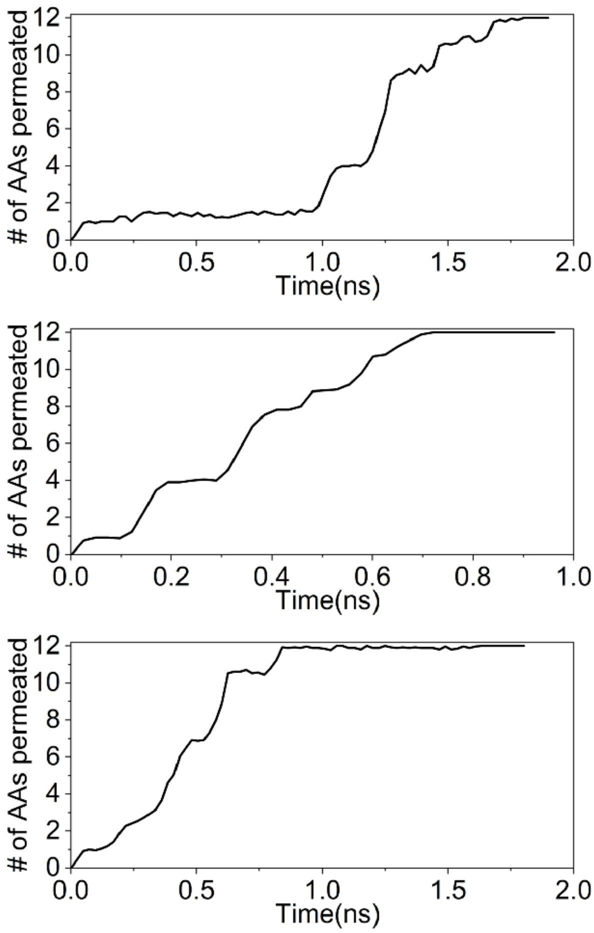


Figure S1. The number of amino acids passing through the nanopore changes with time during the peptide translocation process. The figure shows three different sets of data. In this case, the deceleration system consists of carbon nanotubes.

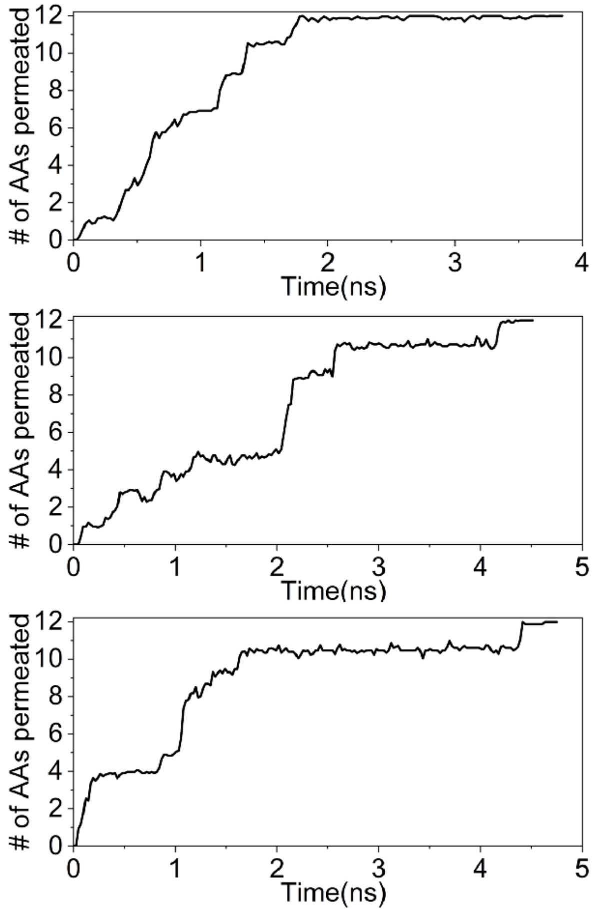


Figure S2. The number of amino acids that pass through the nanopore as a function of time during the translocation process of a polypeptide. Three different sets of data are shown in the figure. In this case, the deceleration system is formed by a carbon nanotube and a gold nanoparticle. The gold nanoparticle is located on the left side of the nanopore, with its rightmost end 7Å away from the center of the nanopore.

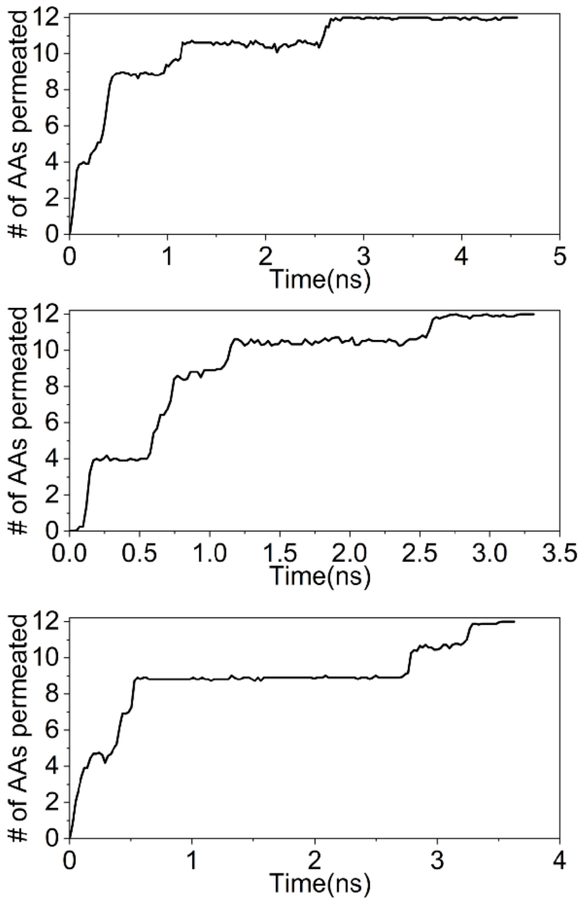


Figure S3. The number of amino acids that pass through the nanopore as a function of time during the translocation process of a polypeptide. Three different sets of data are shown in the figure. In this case, the deceleration system is formed by a carbon nanotube and a gold nanoparticle. The gold nanoparticle is located on the left side of the nanopore, with its rightmost end 4Å away from the center of the nanopore.

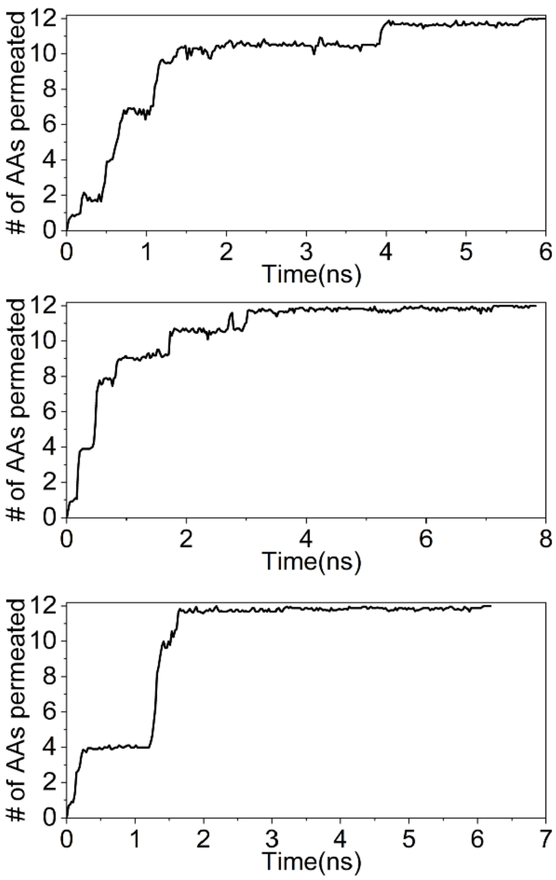


Figure S4. The number of amino acids that pass through the nanopore as a function of time during the translocation process of a polypeptide. Three different sets of data are shown in the figure. In this case, the deceleration system is formed by a carbon nanotube and a gold nanoparticle. The gold nanoparticle is located on the left side of the nanopore, with its rightmost end 1Å away from the center of the nanopore.

From Figures S1 to S4, it can be seen that the translocation time of the peptide is prolonged when gold nanoparticles are added to the decelerating system and as the distance between the gold nanoparticles and the peptide continuously decreases.

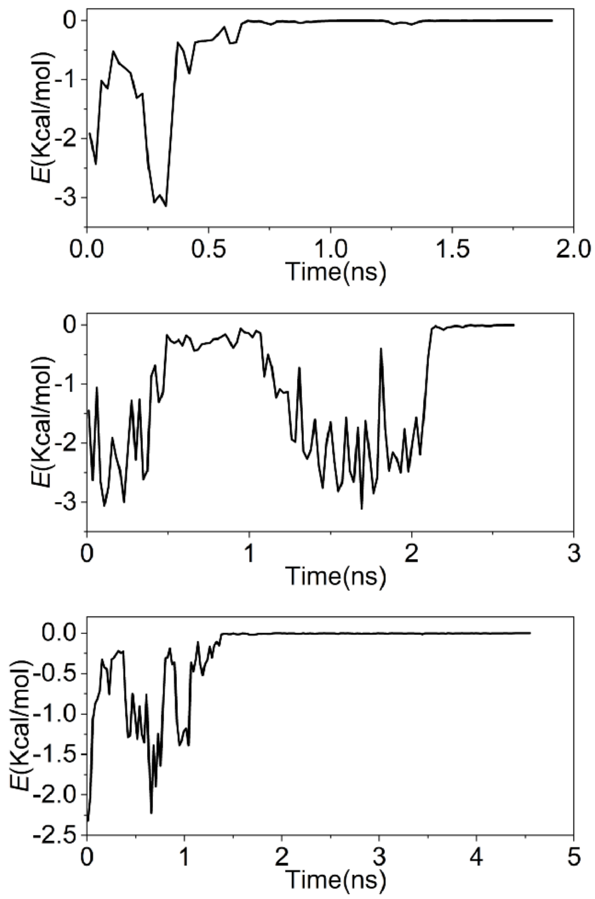


Figure S5. The variation of van der Waals potential energy between peptides and gold nanoparticles over time during the process of peptide translocation. The figure shows three different sets of data. In this case, the deceleration system consists of carbon nanotubes and gold nanoparticles. The gold nanoparticle is located on the left side of the nanopore, with its rightmost end 7Å away from the center of the nanopore.

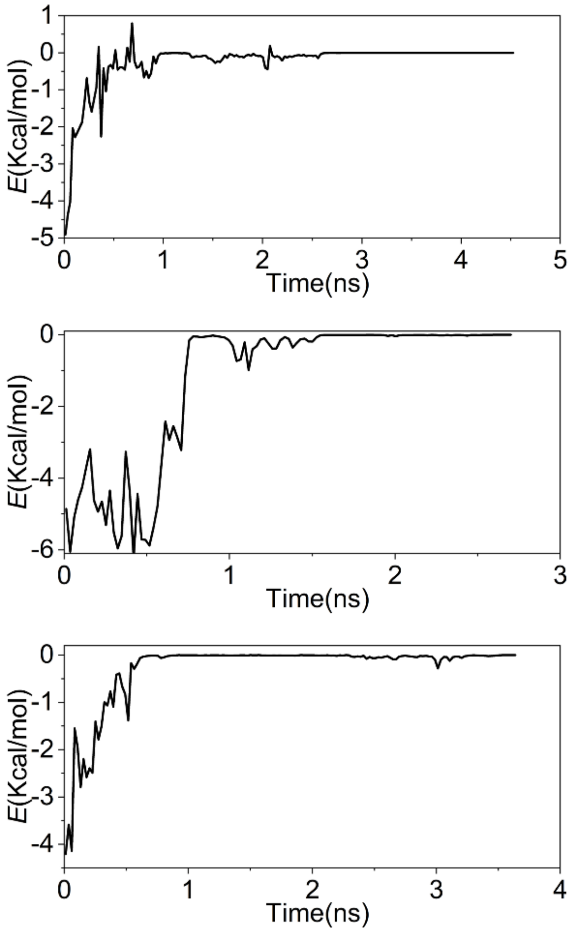


Figure S6. The variation of van der Waals potential energy between peptides and gold nanoparticles over time during the process of peptide translocation. The figure shows three different sets of data. In this case, the deceleration system consists of carbon nanotubes and gold nanoparticles. The gold nanoparticle is located on the left side of the nanopore, with its rightmost end 4Å away from the center of the nanopore.

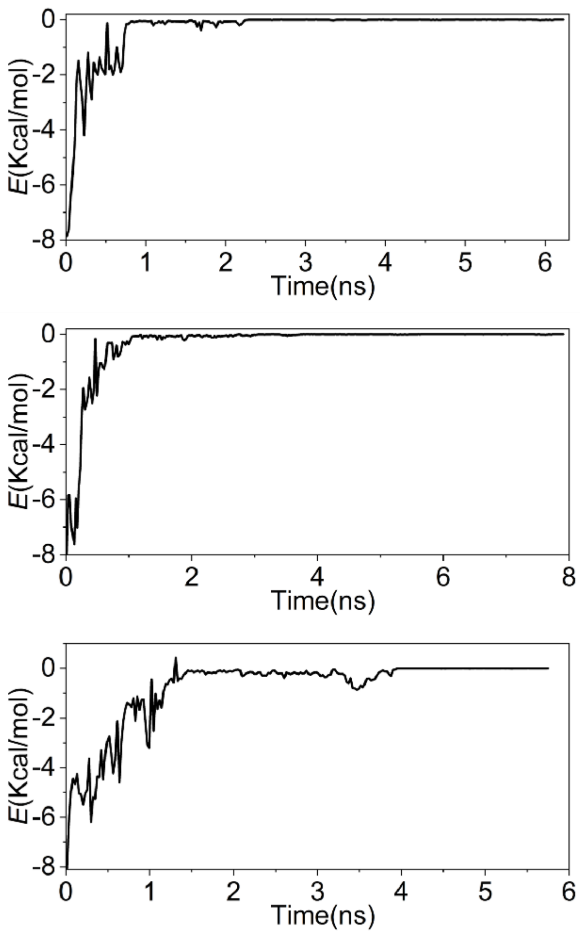


Figure S7. The variation of van der Waals potential energy between peptides and gold nanoparticles over time during the process of peptide translocation. The figure shows three different sets of data. In this case, the deceleration system consists of carbon nanotubes and gold nanoparticles, The gold nanoparticle is located on the left side of the nanopore, with its rightmost end 1Å away from the center of the nanopore.

From Figures S5 to S7, it can be seen that when the distance between the gold nanoparticle and the center of the nanopore changes from 7Å to 1Å, the van der Waals potential energy between the polypeptide and the gold nanoparticle obviously rises.

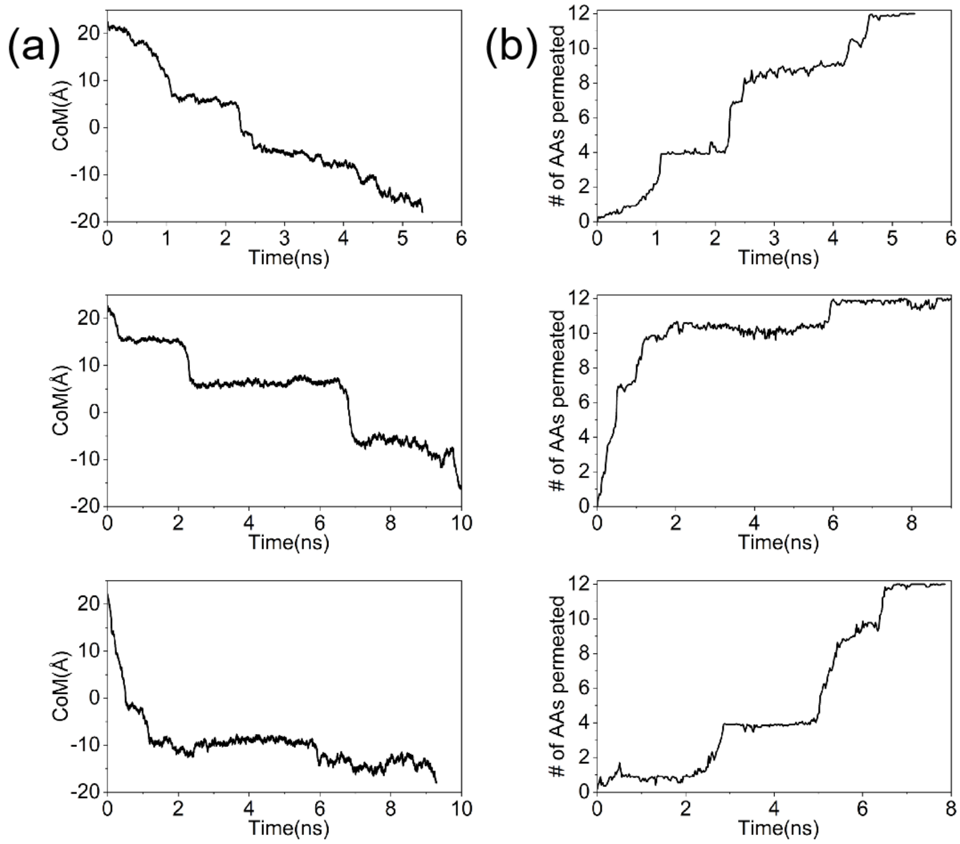


Figure S8. Detailed data of peptides through complex systems. (a) The change in the centroid position of the polypeptide during its translocation through the decelerating system over time. Three different sets of data are shown in the figure. In this case, the decelerating system consists of a carbon nanotube and gold nanoparticles. The gold nanoparticles are located on the right side of the nanopore, with a distance of 2Å between their rightmost end and the center of the nanopore. (b) The number of amino acids passing through the nanopore during the polypeptide translocation process over time. The system settings and data sources are the same as in (a).

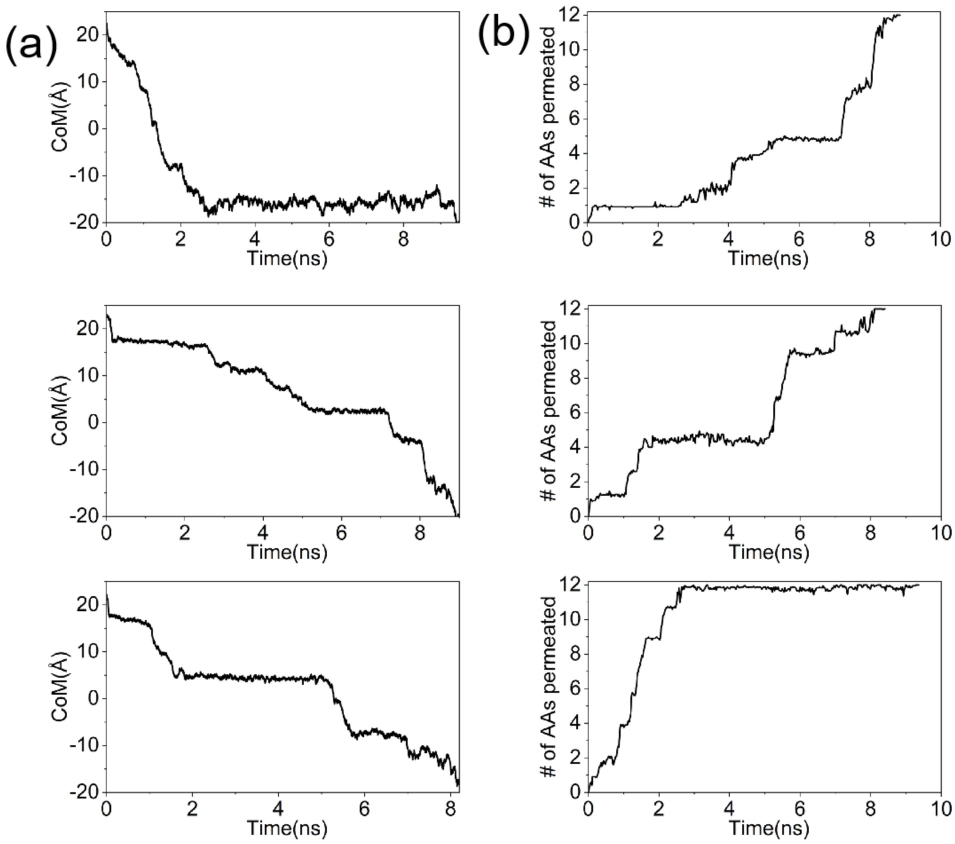


Figure S9. Detailed data of peptides through complex systems. (a) The change in the centroid position of the polypeptide during its translocation through the decelerating system over time. Three different sets of data are shown in the figure. In this case, the decelerating system consists of a carbon nanotube and gold nanoparticles. The gold nanoparticles are located on the right side of the nanopore, with a distance of 4Å between their rightmost end and the center of the nanopore. (b) The number of amino acids passing through the nanopore during the polypeptide translocation process over time. The system settings and data sources are the same as in (a).

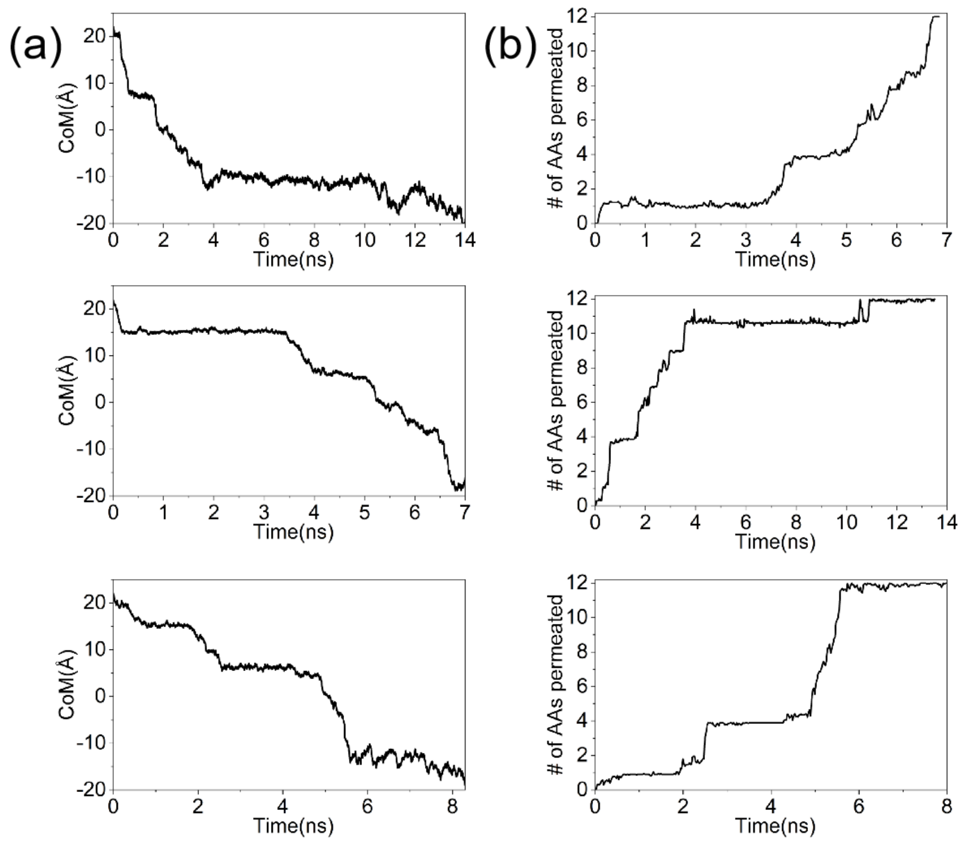


Figure S10. Detailed data of peptides through complex systems. (a) The change in the centroid position of the polypeptide during its translocation through the decelerating system over time. Three different sets of data are shown in the figure. In this case, the decelerating system consists of a carbon nanotube and gold nanoparticles. The gold nanoparticles are located on the right side of the nanopore, with a distance of 6Å between their rightmost end and the center of the nanopore. (b) The number of amino acids passing through the nanopore during the polypeptide translocation process over time. The system settings and data sources are the same as in (a).

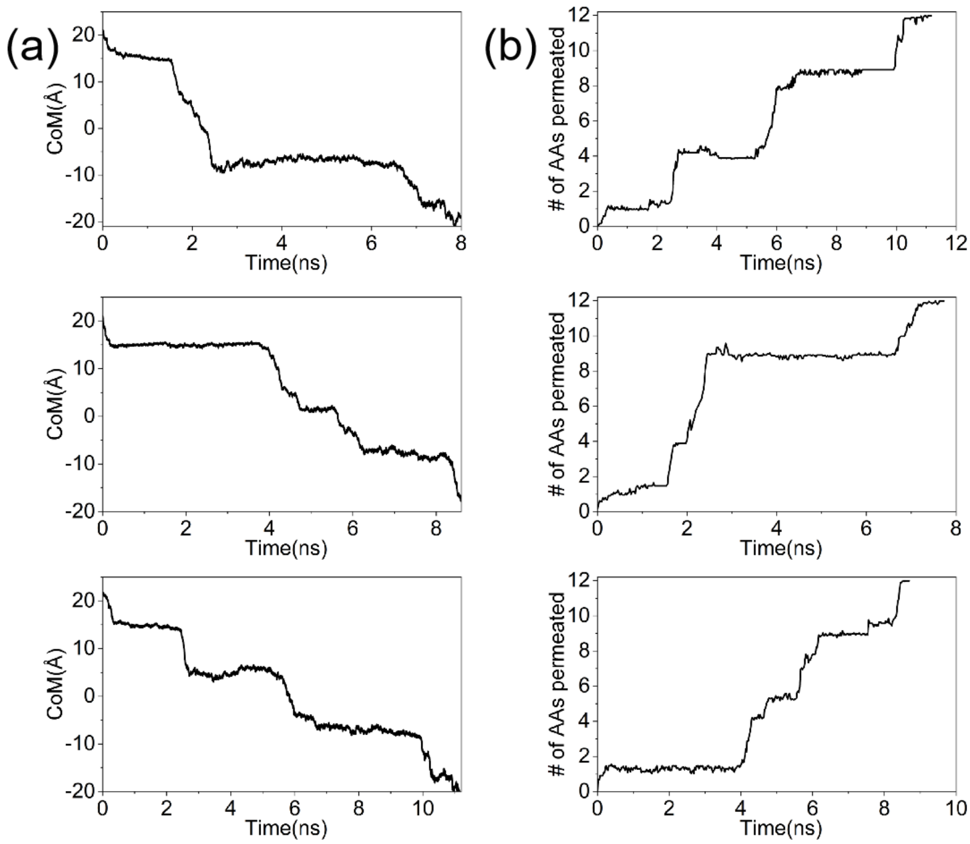


Figure S11. Detailed data of peptides through complex systems. (a) The change in the centroid position of the polypeptide during its translocation through the decelerating system over time. Three different sets of data are shown in the figure. In this case, the decelerating system consists of a carbon nanotube and gold nanoparticles. The gold nanoparticles are located on the right side of the nanopore, with a distance of 8Å between their rightmost end and the center of the nanopore. (b) The number of amino acids passing through the nanopore during the polypeptide translocation process over time. The system settings and data sources are the same as in (a).

It can be seen from Figures S8–S11 that the time of peptide translocation through the composite system was further prolonged with the continuous deepening of gold nanoparticles.

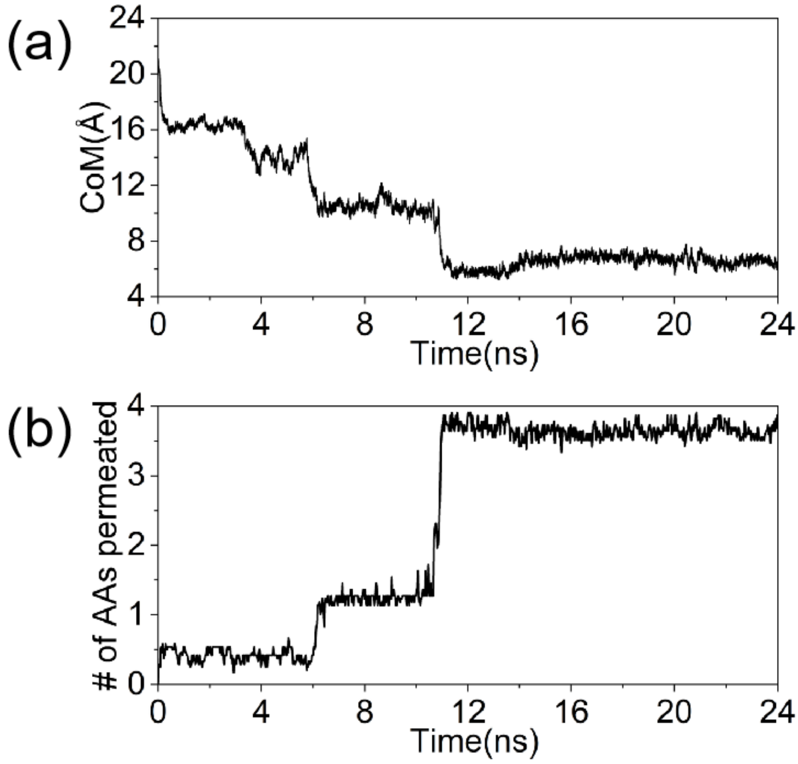


Figure S12. MD simulation of peptide translocation in a composite system when the gold nanoparticle is located too deep. (a) The change in the centroid position over time during the peptide translocation process. In this case, the decelerating system consists of a carbon nanotube and a gold nanoparticle. The gold nanoparticle is located on the right side of the nanopore, with a distance of 10 angstroms between its rightmost end and the center of the nanopore. (b) The change in the number of amino acids passing through the nanopore over time during the peptide translocation process. The system settings and data sources are the same as in (a).

From the position of the center of mass and the number of amino acids passing through the nanopore when the polypeptide is in a stable state , it can be seen that the polypeptide has not all passed through the composite system.

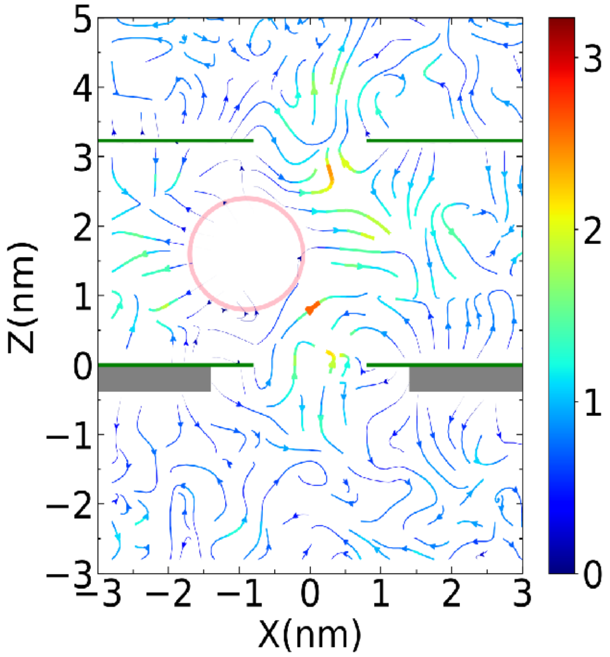


Figure S13. Stationary local densities of the ionic contributions to the total current in the YOZ plane for the model system consisting of a carbon nanotube and a charged gold nanoparticle. The arrows indicate the direction of the local fluxes, and the color indicates the magnitude of the local fluxes. The figures were calculated from 24 ns long MD trajectories sampled at a frequency of 4.8 ps.

From the figure, it can be seen that the total flow field direction is upward, which can reduce the speed of peptide translocation through the composite system to a certain extent.

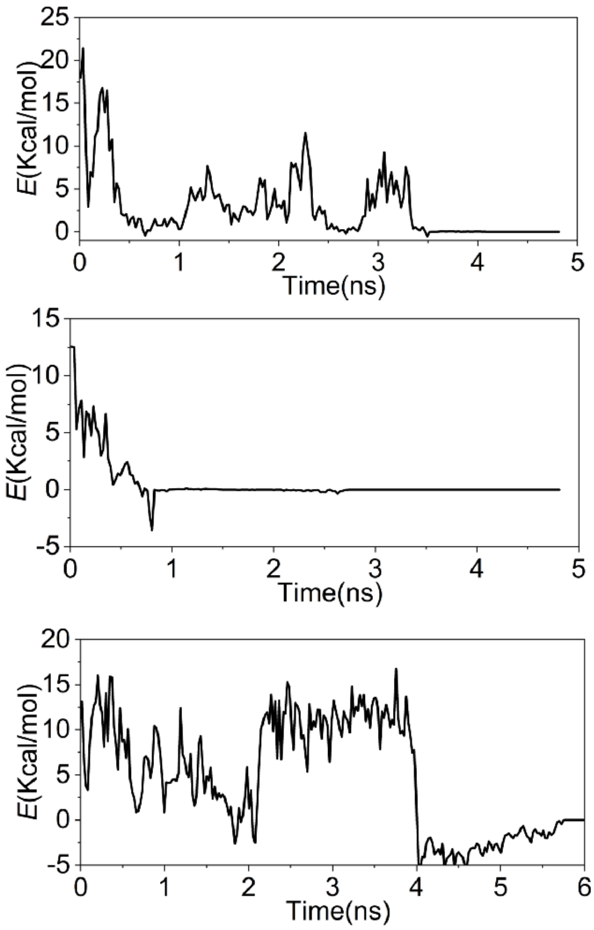


Figure S14. The electrostatic potential energy of the peptide and gold nanoparticle changes with time during the translocation process. Three different sets of data are shown in the figure. In this case, the ratcheting system is composed of a carbon nanotube and a charged gold nanoparticle. The charged gold nanoparticle is located on the left side of the nanopore, and the distance between its rightmost end and the center of the nanopore is 7Å.

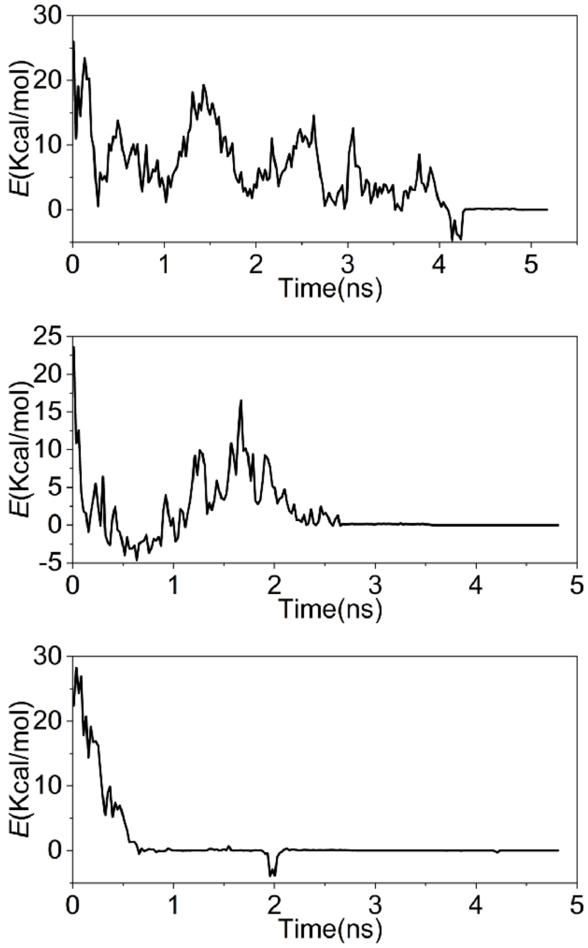


Figure S15. The electrostatic potential energy of the peptide and gold nanoparticle changes with time during the translocation process. Three different sets of data are shown in the figure. In this case, the ratcheting system is composed of a carbon nanotube and a charged gold nanoparticle. The charged gold nanoparticle is located on the left side of the nanopore, and the distance between its rightmost end and the center of the nanopore is 5Å.

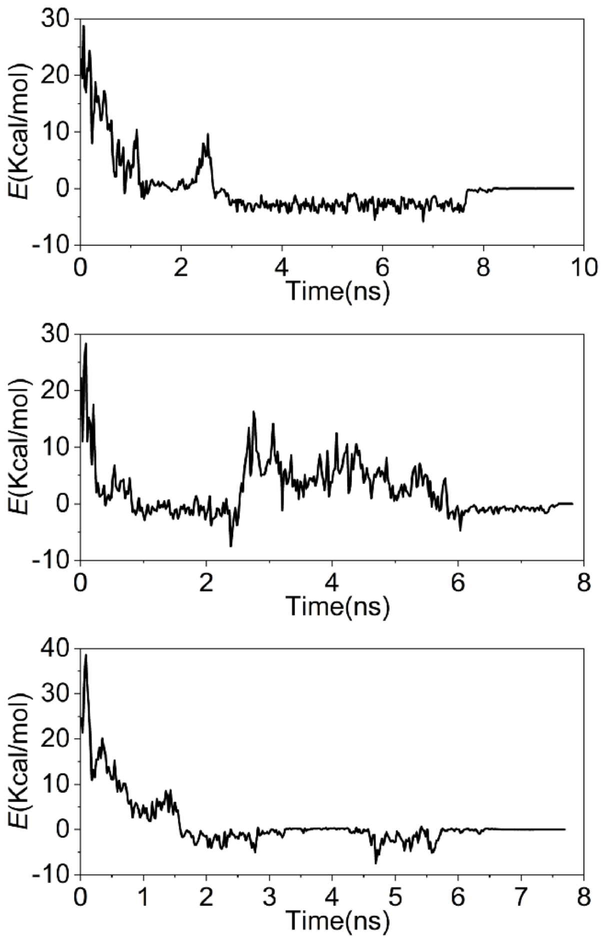


Figure S16. The electrostatic potential energy of the peptide and gold nanoparticle changes with time during the translocation process. Three different sets of data are shown in the figure. In this case, the ratcheting system is composed of a carbon nanotube and a charged gold nanoparticle. The charged gold nanoparticle is located on the left side of the nanopore, and the distance between its rightmost end and the center of the nanopore is 3Å.

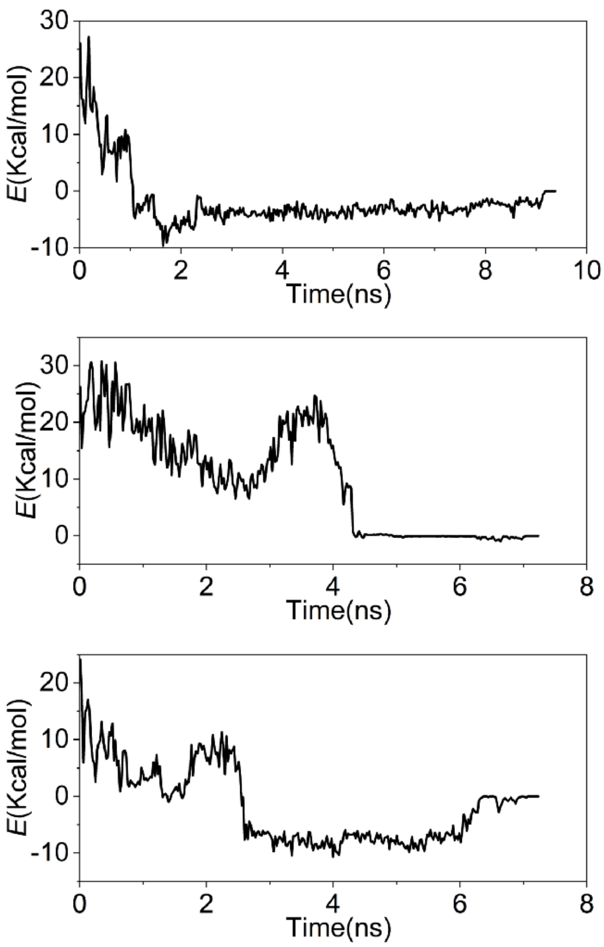


Figure S17. The electrostatic potential energy of the peptide and gold nanoparticle changes with time during the translocation process. Three different sets of data are shown in the figure. In this case, the ratcheting system is composed of a carbon nanotube and a charged gold nanoparticle. The charged gold nanoparticle is located on the left side of the nanopore, and the distance between its rightmost end and the center of the nanopore is 1Å.

From Figures S14 to S17, it can be seen that when the distance between the gold nanoparticle and the center of the nanopore changes from 7Å to 3Å, the electrostatic potential energy between the polypeptide and the gold nanoparticle increases obviously. When the distance between the gold nanoparticle and the center of the nanopore changes from 3Å to 1Å, the electrostatic potential energy between the polypeptide and the gold nanoparticle remains basically unchanged.

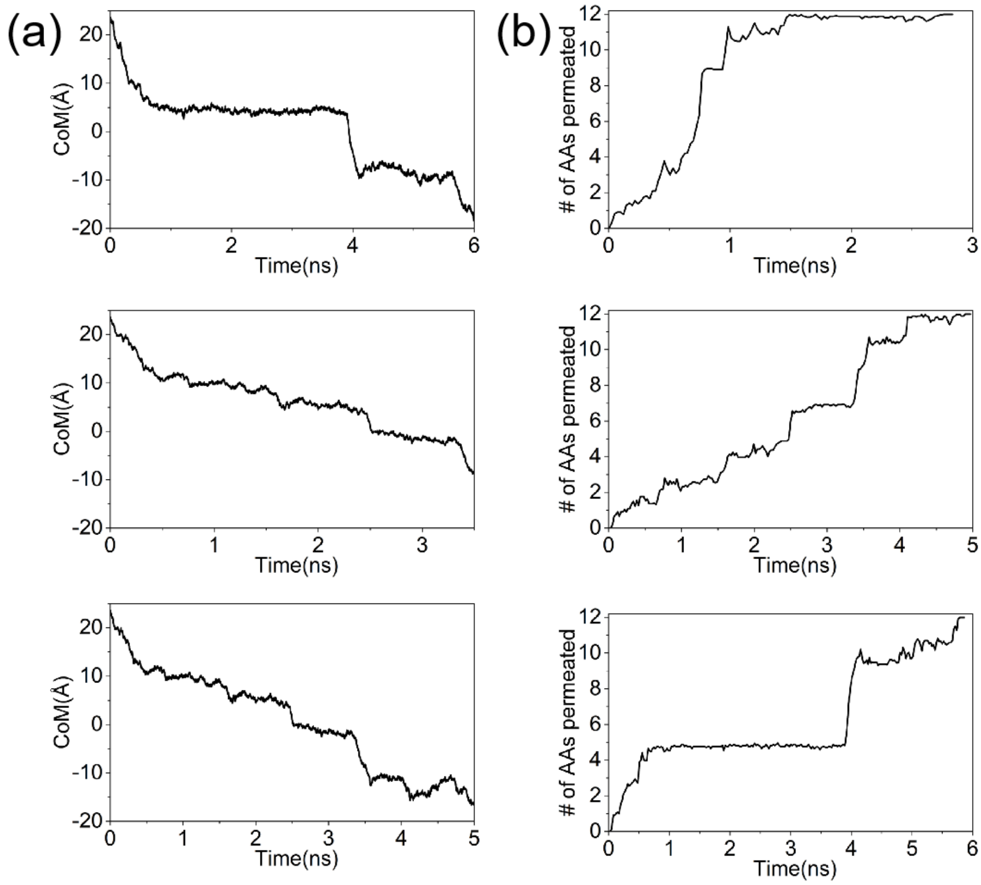


Figure S18. Detailed data of the peptide translocation through the complex system. (a) The change in the position of the center of mass with time during the process of peptide translocation through the decelerating system. Three sets of different data are shown in the figure. In this case, the decelerating system is composed of a carbon nanotube and a charged gold nanoparticle. The charged gold nanoparticle is located on the left side of the nanopore, and the distance between its rightmost end and the center of the nanopore is 7Å. (b) The change in the number of amino acids passing through the nanopore with time during the peptide translocation process. The system settings and data sources are the same as those in (a).

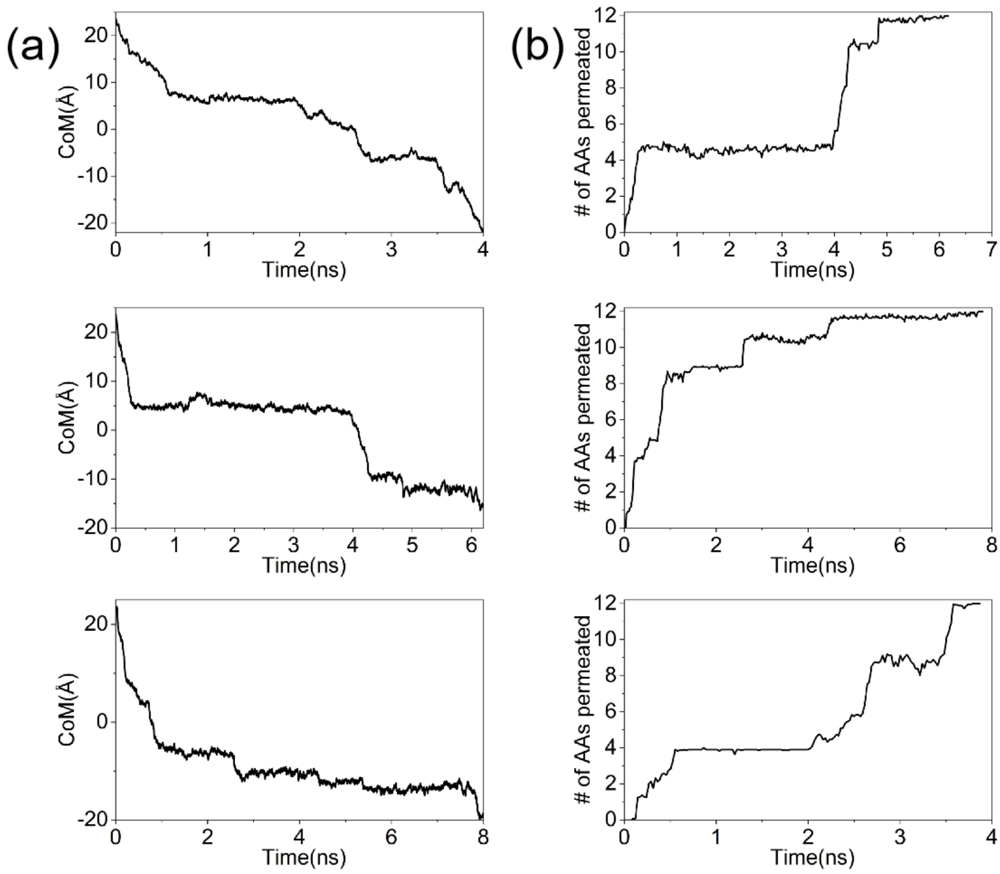


Figure S19. Detailed data of the peptide translocation through the complex system. (a) The change in the position of the center of mass with time during the process of peptide translocation through the decelerating system. Three sets of different data are shown in the figure. In this case, the decelerating system is composed of a carbon nanotube and a charged gold nanoparticle. The charged gold nanoparticle is located on the left side of the nanopore, and the distance between its rightmost end and the center of the nanopore is 5Å. (b) The change in the number of amino acids passing through the nanopore with time during the peptide translocation process. The system settings and data sources are the same as those in (a).

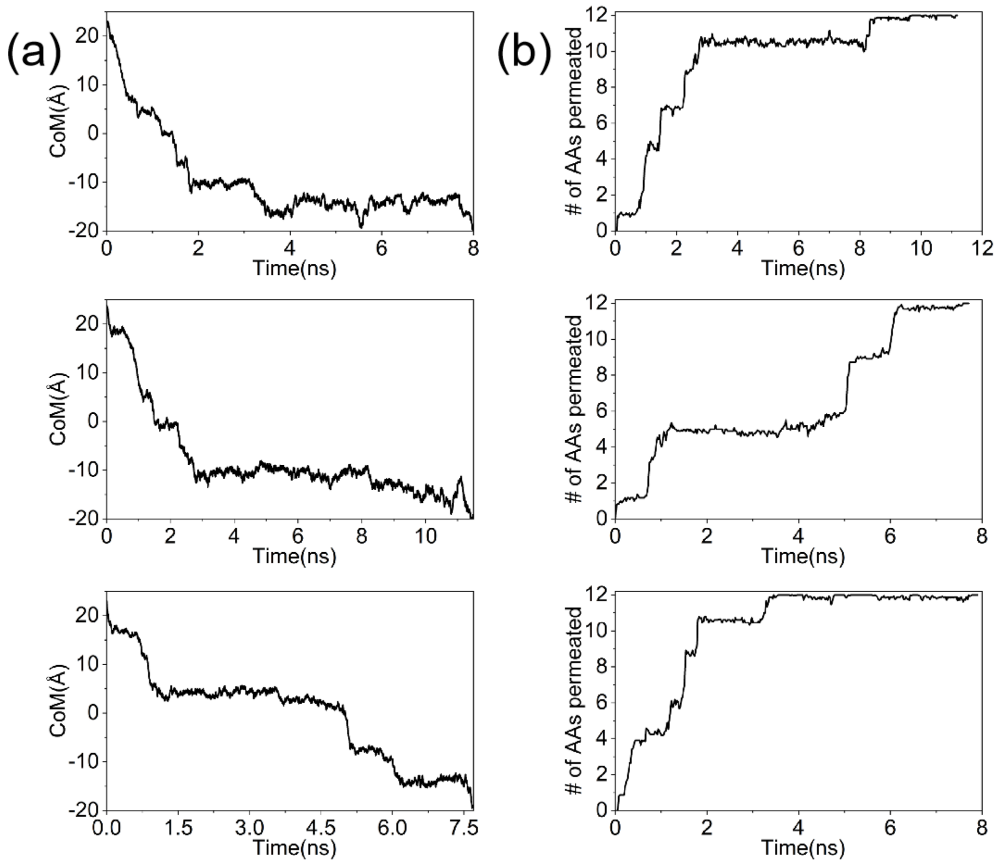


Figure S20. Detailed data of the peptide translocation through the complex system. (a) The change in the position of the center of mass with time during the process of peptide translocation through the decelerating system. Three sets of different data are shown in the figure. In this case, the decelerating system is composed of a carbon nanotube and a charged gold nanoparticle. The charged gold nanoparticle is located on the left side of the nanopore, and the distance between its rightmost end and the center of the nanopore is 3Å. (b) The change in the number of amino acids passing through the nanopore with time during the peptide translocation process. The system settings and data sources are the same as those in (a).

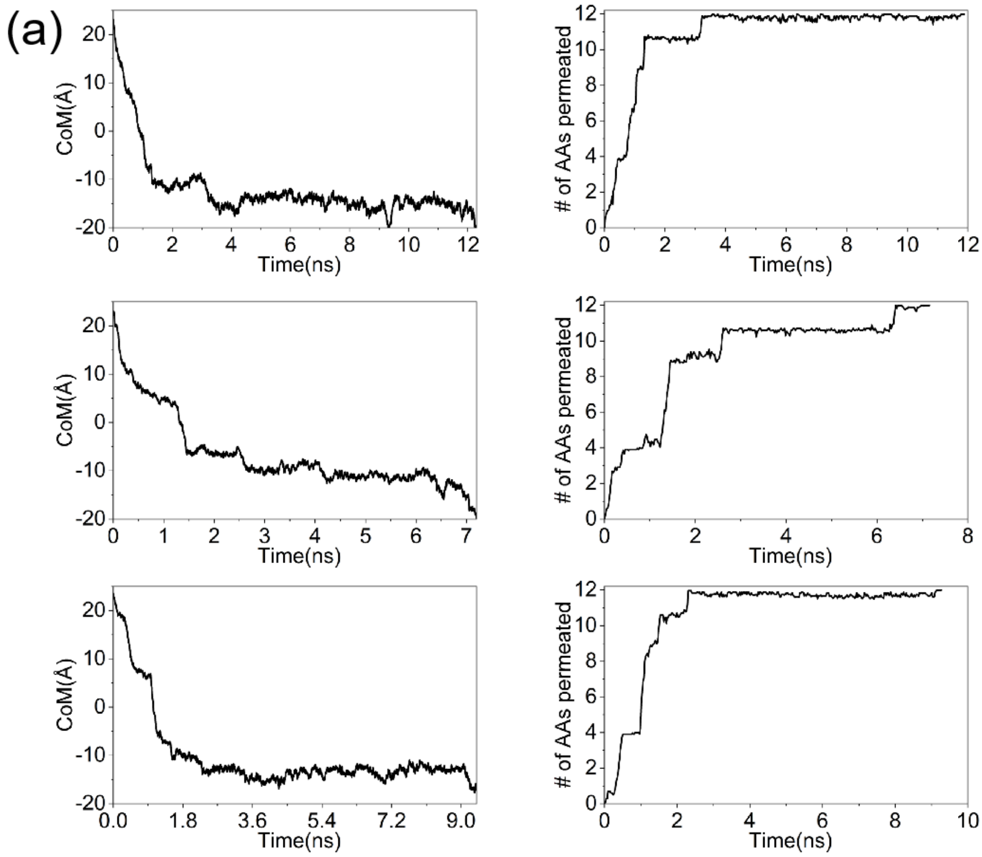


Figure S21. Detailed data of the peptide translocation through the complex system. (a) The change in the position of the center of mass with time during the process of peptide translocation through the decelerating system. Three sets of different data are shown in the figure. In this case, the decelerating system is composed of a carbon nanotube and a charged gold nanoparticle. The charged gold nanoparticle is located on the left side of the nanopore, and the distance between its rightmost end and the center of the nanopore is 1Å. (b) The change in the number of amino acids passing through the nanopore with time during the peptide translocation process. The system settings and data sources are the same as those in (a).

From Figure S18 to Figure S21, it can be seen that as the distance between charged gold nanoparticles and peptides increases, the translocation time of peptides also prolongs.

Table S1 Parameters used for gold nanoparticle[1]

| Atom type | Bond lengths | Angles | Lennard-Jones potential | | CHARMM force field parameters | |
|---|---|---|---|---|---|---|
| | $d_{1,2}$ (Å) | $\theta_{1,2}$ (°) | $\epsilon$ (kcal/mol) | $\sigma$ (Å) | $\epsilon$ (kcal/mol) | $R_{min}/2$ (Å) |
| Au | 2.884 | 180 | 0.039 | 2.934 | 0.039 | 1.647 |

# References

1. Q. Pu, Y. S. Leng, X. C. Zhao and P. T. Cummings, *Nanotechnology*, 2007, **18**, 424007.