Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Different Platinum Crystal Surfaces Show Very Distinct Protein Denaturation Capability

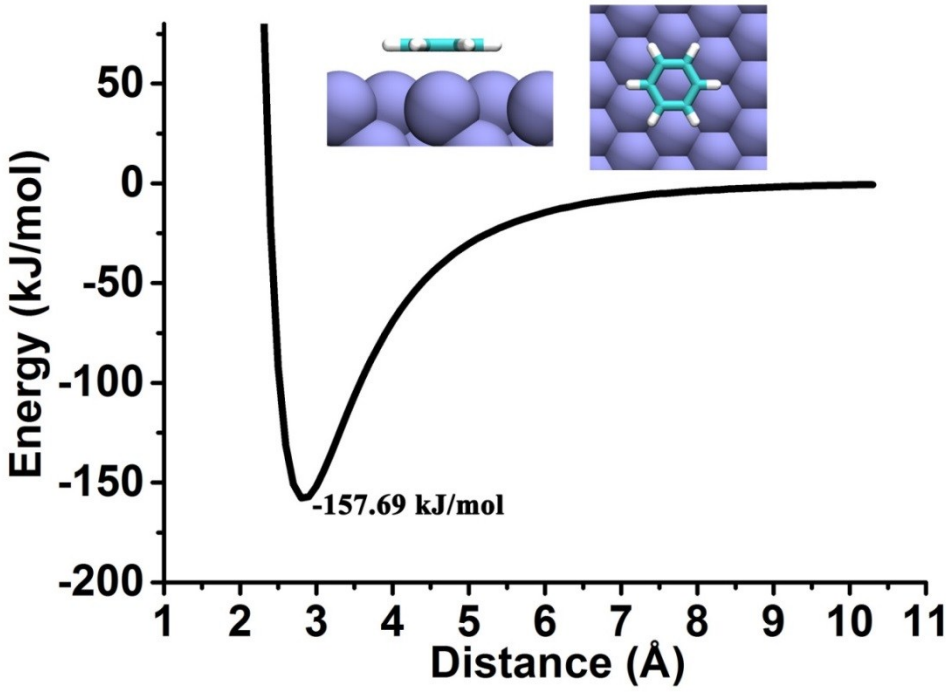

Figure S1. The adsorption energy profile of a benzene molecule approaching the Pt(111) surface.

Table S1. Comparison of adsorption energy (E_{ad}) among DFT calculations, MD simulation and experimental data for benzene on Pt(111).

System	Method	E_{ad} (kJ/mol)
	optB88-vdW	177.53[a]
	Experiment	151.48-184.29[b]
	This work	**157.69**

a. The adsorption energy predicted by DFT calculations accounting for vdW interaction.[1] b. The heat of adsorption measured with calorimetry.[2]

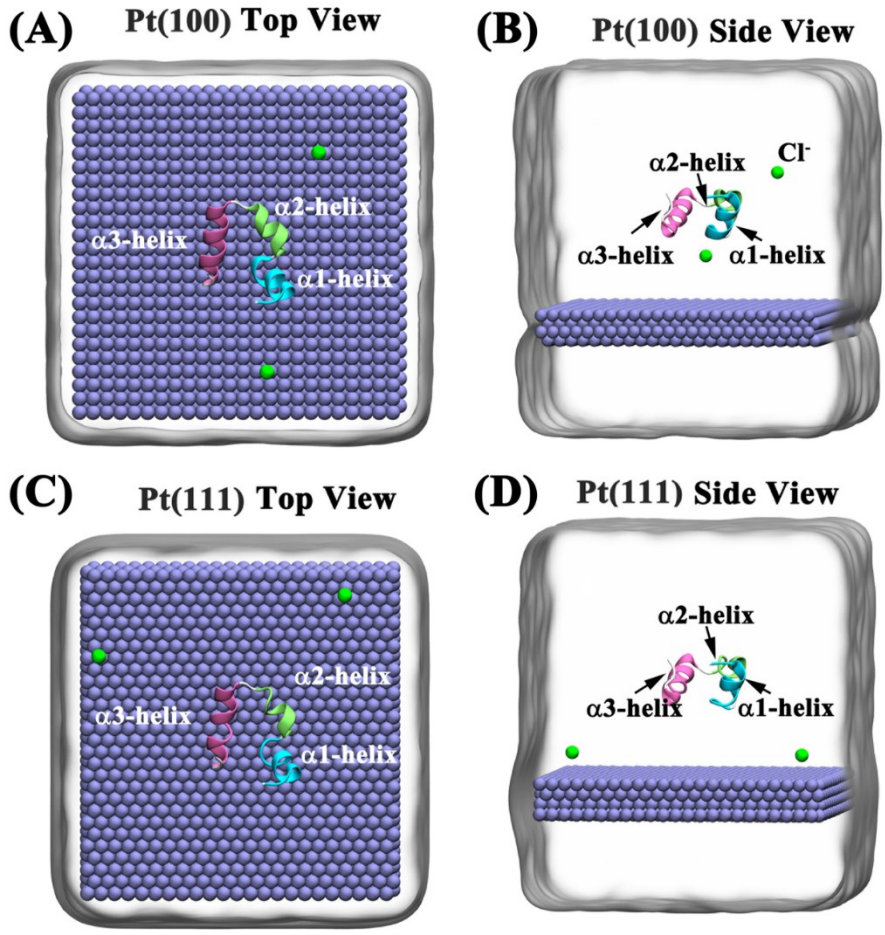

Figure S2. Top and side views of the initial configurations of the HP35 protein on Pt(100) (A and B) and Pt(111) (C and D) surfaces, respectively. The water box is rendered here as a transparent sliver surface. The platinum atoms and chloride ions are shown as van der Waals spheres, colored by ice blue and green, respectively. The HP35 protein is represented by a new cartoon model and colored differently based on the helix indexes: α1 (residues 43–52), α2 (residues 54–61) and α3 (residues 63–74) helices are colored by blue, green, and pink, respectively.

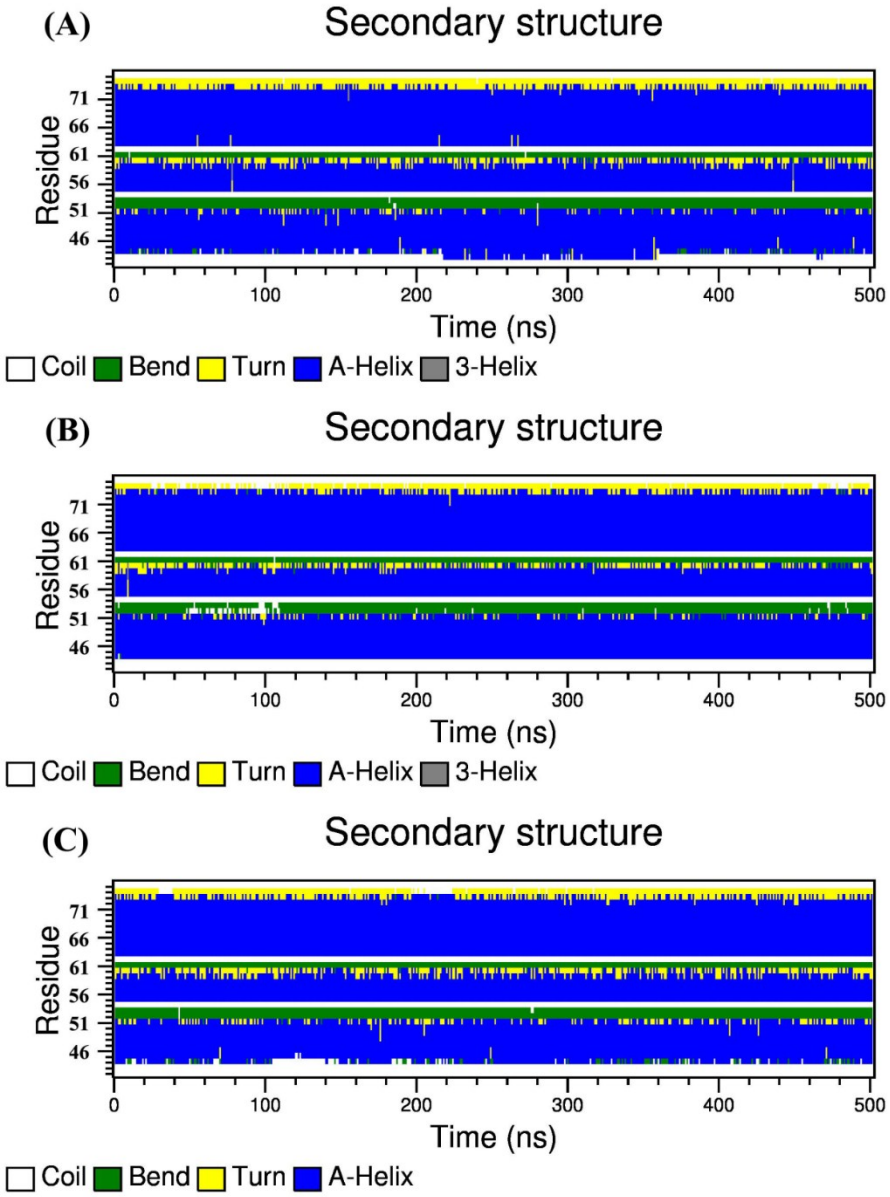

Figure S3. Time evolution of the secondary structure of the HP35 protein in pure water in three independent trajectories. Each trajectory is shown in the panels from A to C, respectively.

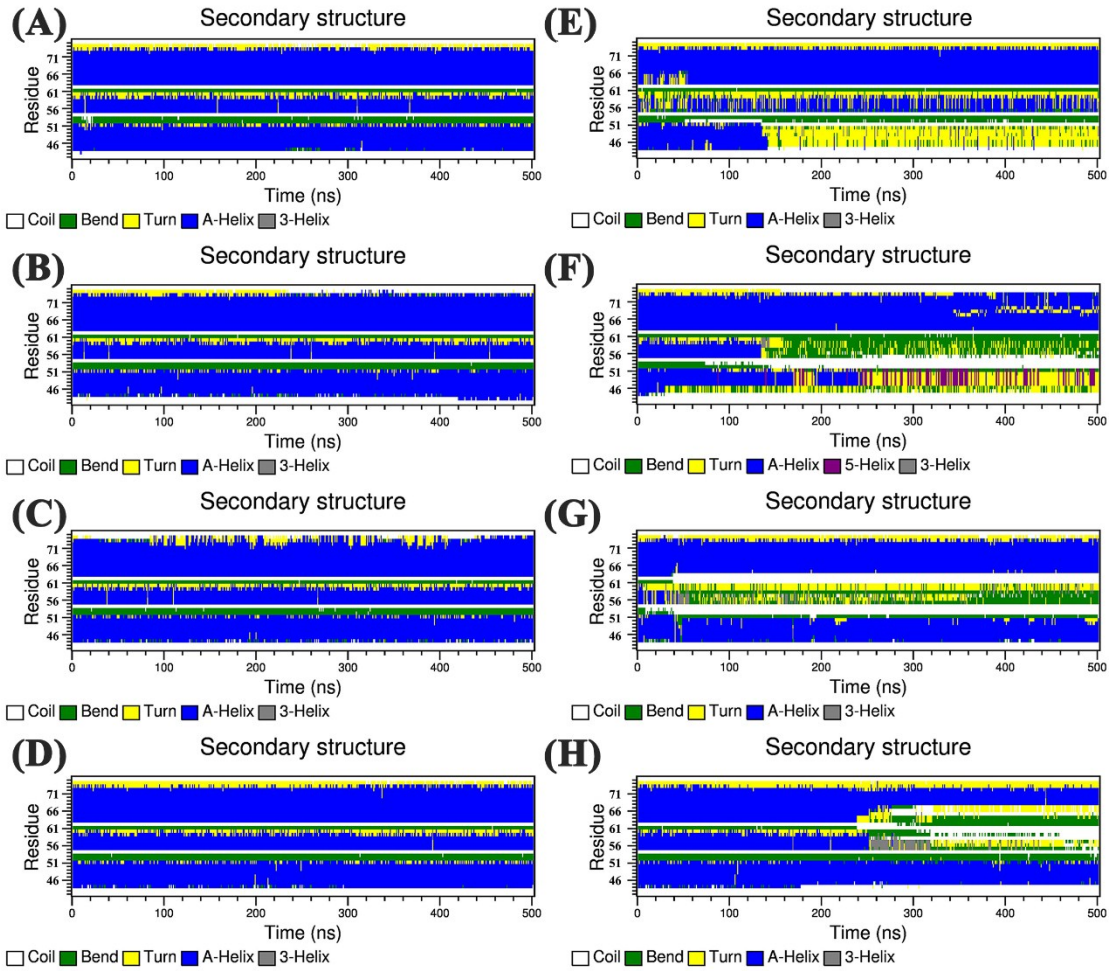

Figure S4. Time evolution of the secondary structure of the HP35 at the Pt(100) surface (A-D) and Pt(111) surface (E-H) in the four other independent trajectories. Each trajectory is shown in each panel.

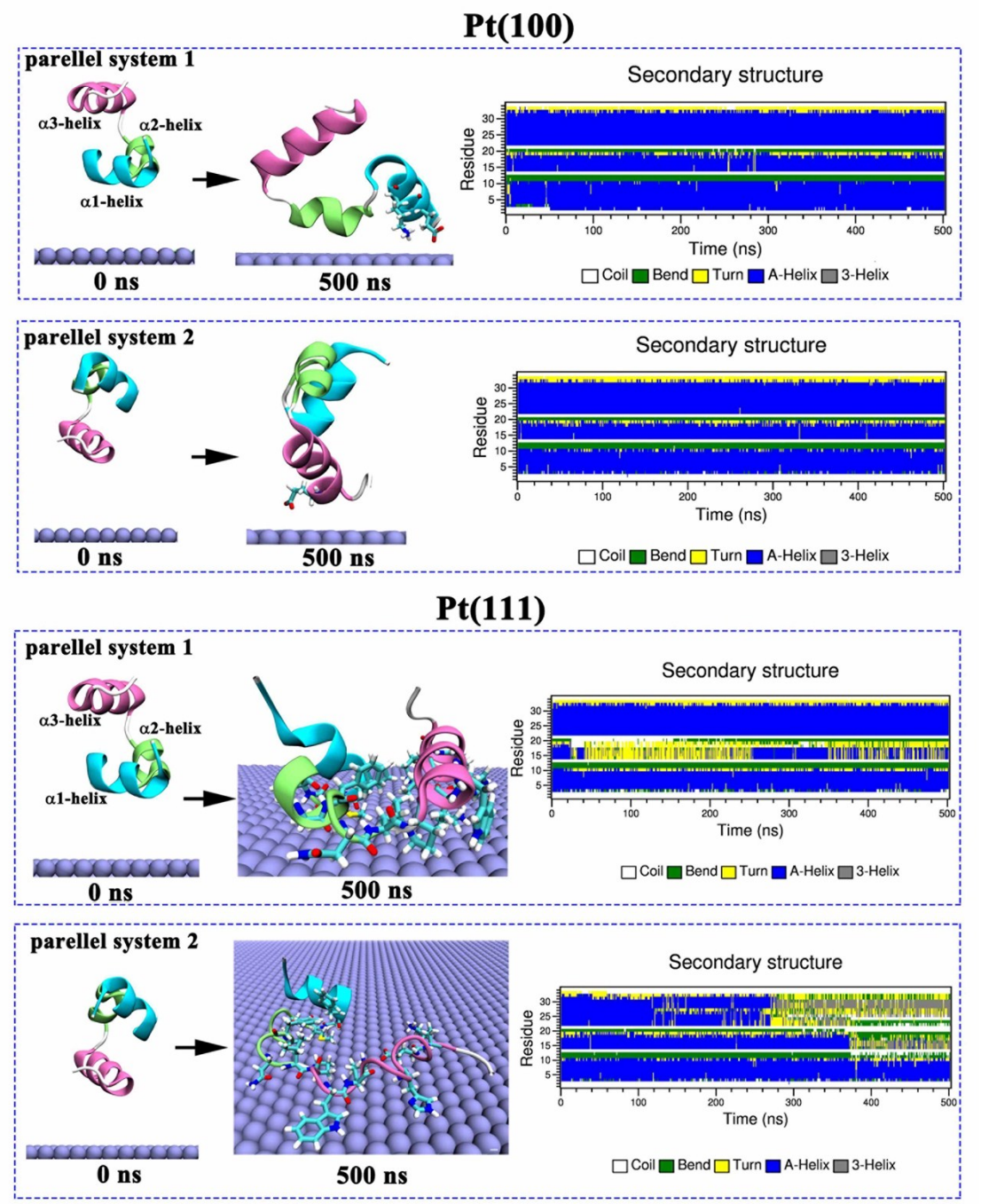

Fig S5. The initial and final configurations of protein-Pt surfaces complex, and time evolution of the secondary structure of the protein in the two additional parallel simulations (with different initial configurations) for both Pt(100) and Pt(111) systems.

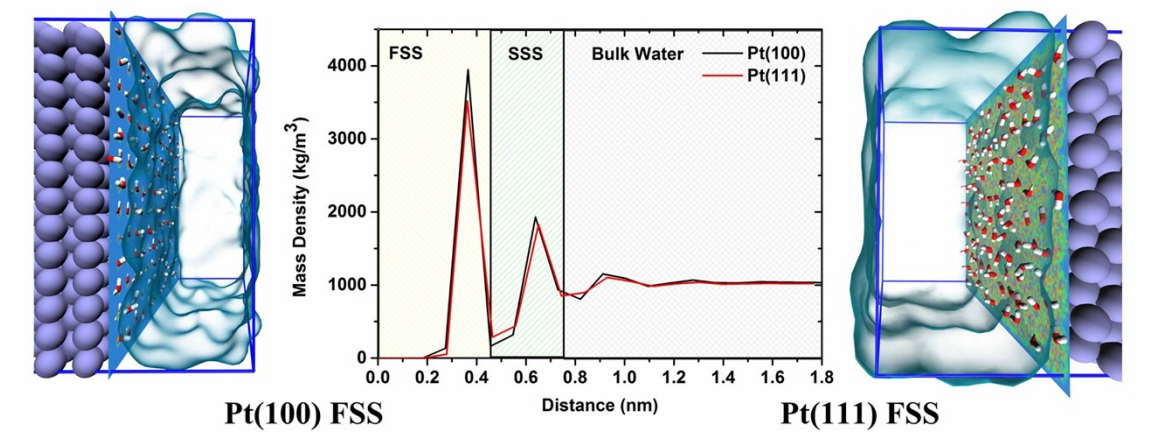

Figure S6. The first solvation shell (FSS) and second solvation shell (SSS) are defined based on the distribution of water density along the normal of the two Pt surfaces. The distances from the Pt surface, for the upper boundaries of the FSS and SSS are located at the first (~0.45 nm) and second minimum points (~ 0.74 nm) in the water-density-distribution curve. The positions of the two minimum points are almost identical in two Pt surfaces.

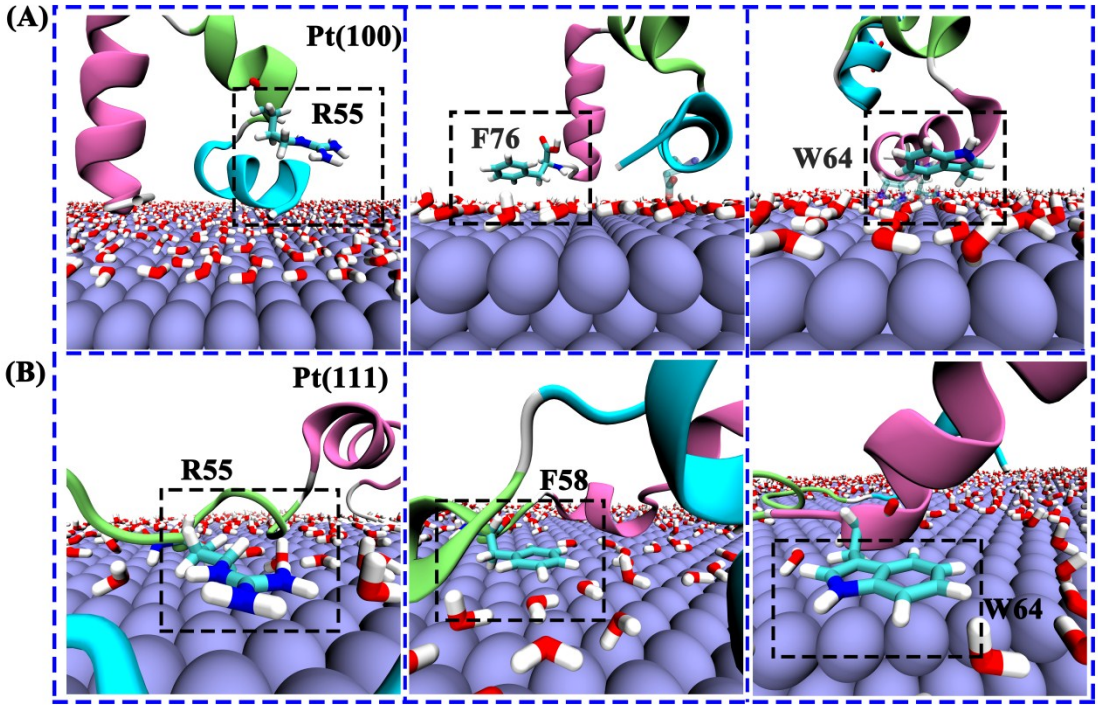

Figure S7. Snapshots of different configurations of R55, F76, W64, and F58 of the HP35 protein adsorbed onto the Pt(100) and Pt(111) surfaces. (A) R55, F76 and W64 are isolated from the Pt(100) surface by the water monolayer in the FSS. (B) R55, F58 and W64 make direct contact with the Pt(111) surface.

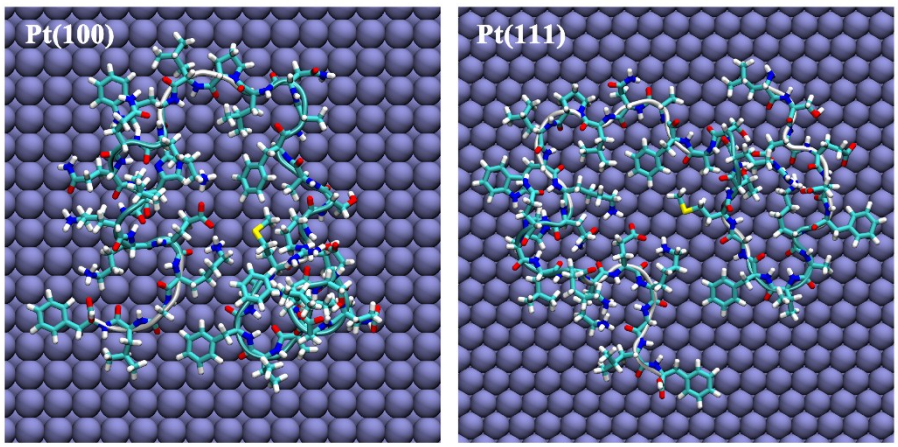

Figure S8. The HP35 protein denatured at Pt(100) (left panel) and Pt(111) surface (right panel) when water is absent. The final snapshots of the HP35 at t = 500 ns on to Pt crystal surfaces.

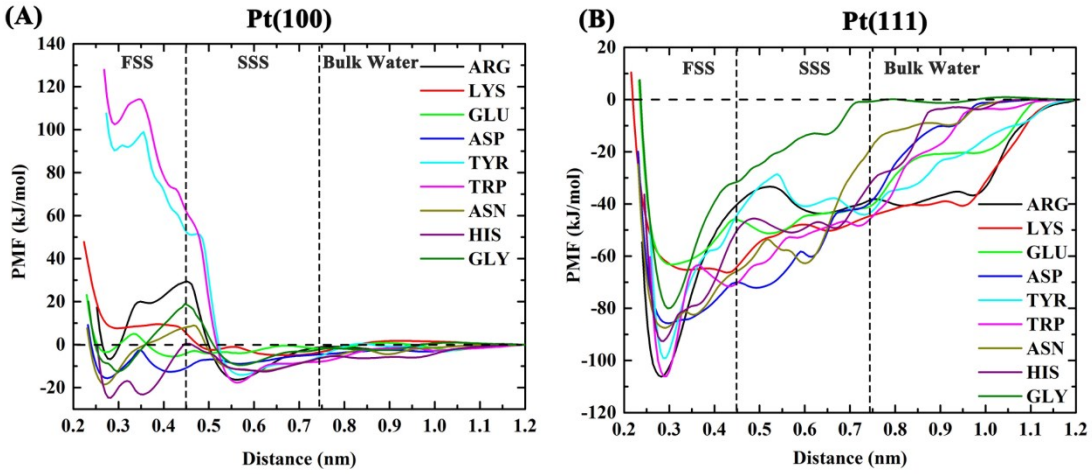

Figure S9. The PMF of the adsorption of some amino acids onto the (A) Pt(100) and (B) Pt(111) surfaces.

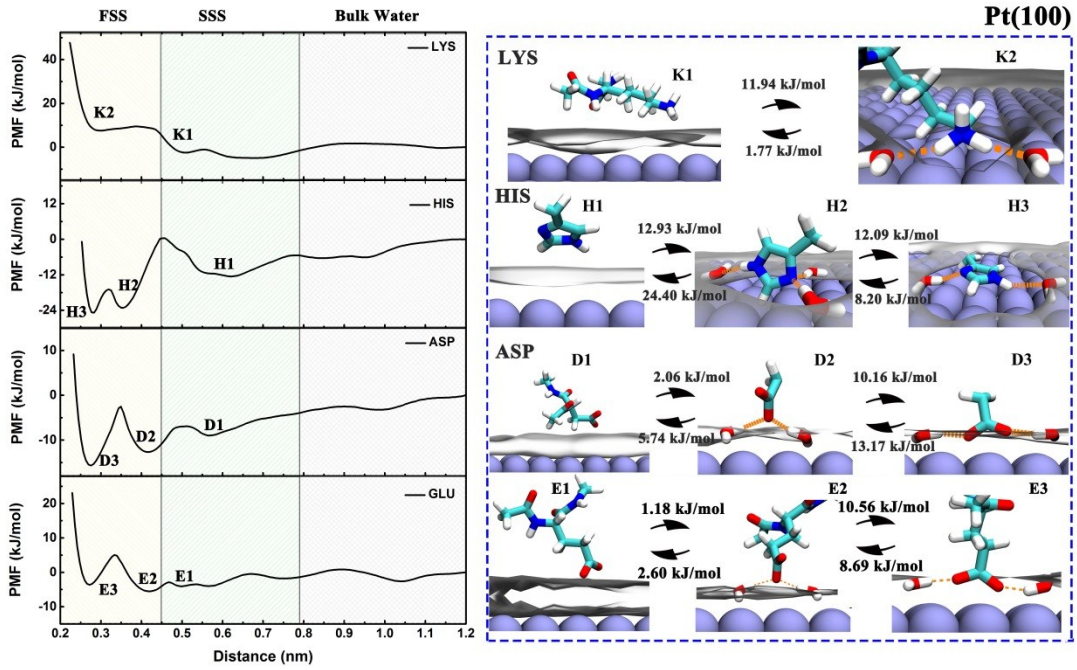

Figure S10. The PMF of the adsorption of Lys, His, Asp and Glu onto the Pt(100) surface (left panel), and some representative configurations, taken from the windows at the free energy minima in the PMF (right panel).

1 W. Liu, J. Carrasco, B. Santra, A. Michaelides, M. Scheffler and A. Tkatchenko, *Phys. Rev. B*, 2012, **86**, 245405.

2 H. Ihm, H. M. Ajo, J. M. Gottfried, P. Bera and C. T. Campbell, *J. Phys. Chem. B*, 2004, **108**, 14627-14633.