Supporting Information For

Facet-regulated Adhesion of Double-stranded DNA on Palladium Surfaces

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Table S1. Simulation details of the four systems in this study.

	Pd(100)-dsDNA	Pd(111)-dsDNA	Pd(100)-water	Pd(111)-water
Box size (nm^3)	10.11×10.11×9.51	9.90×9.53×9.65	10.11×10.11×5.52	9.90×9.53×5.60
Number of water molecules	31,535	29,017	18,432	16,847
Number of potassium ions	92	85	0	0
Number of chloride ions	62	55	0	0
Length of production runs (ns)	500	500	10	10
Number of trajectories	3	3	1	1
Collected time step (ps)	50	50	2	2

Table S2. The direct vdW energy between deoxyadenosine and Pd sheet.

	Pd(100)-A position (i)	Pd(100)-A position (ii)	Pd(111)-A position (iii)
Pd-A vdW (kcal/mol)	-7.9±0.5	-72.7±2.0	-75.7±1.7

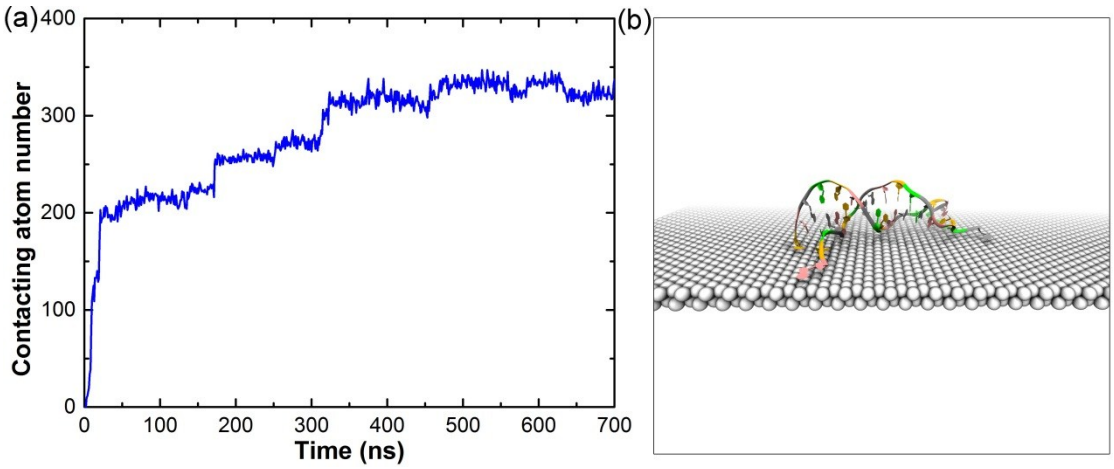

Figure S1. Verification the convergence of the simulation on Pd(111). (a) Time evolution of heavy atom contact number between dsDNA to the Pd(111) surface in an extended simulation (to 700 ns) to show the convergence of the simulation. (b) The final binding conformation at 700 ns.

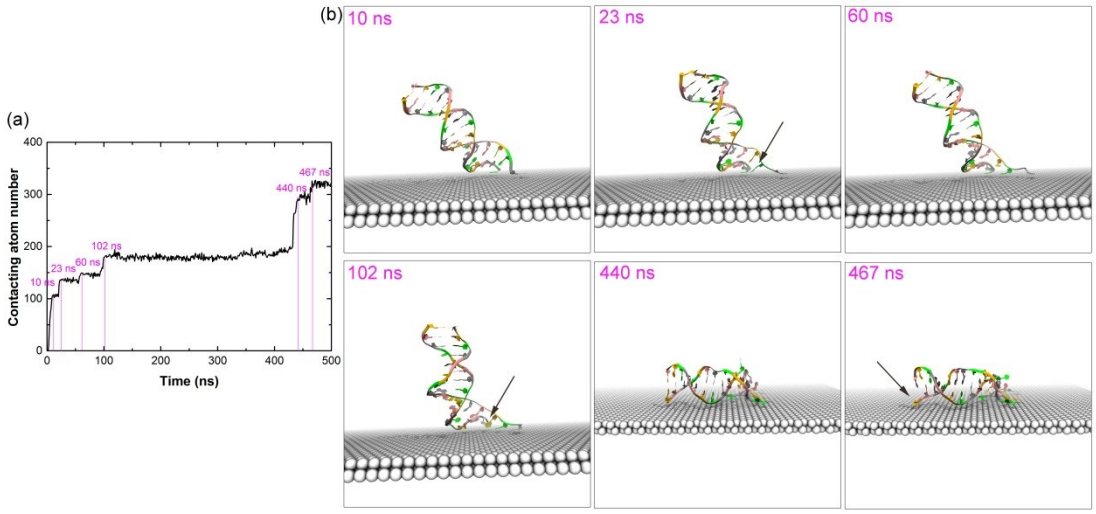

Figure S2. Step-wise binding pattern of dsDNA to Pd(111). (a) A typical trajectory to shows time evolution of the heavy atom contact number of dsDNA binding to Pd(111). (b) Some snapshots of dsDNA binding to Pd(111) in some key time points.

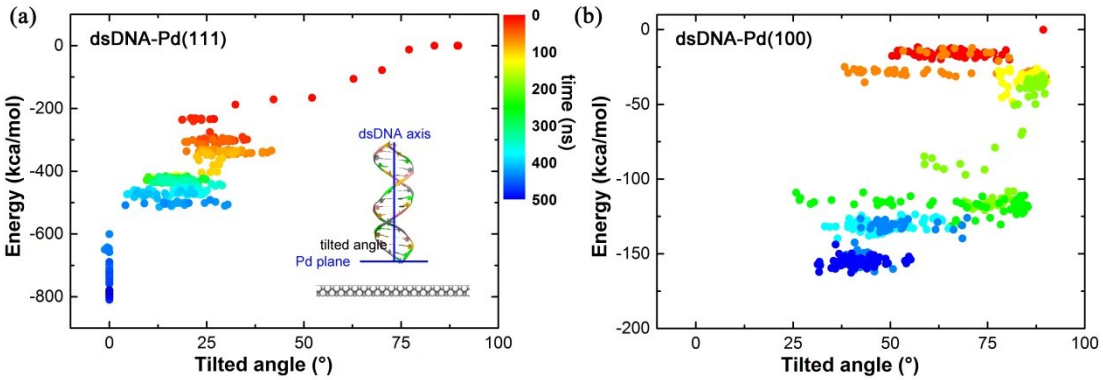

Figure S3. The dsDNA-Pd surface tilted angle versus dsDNA-Pd interaction energy. (a) for Pd(111), and (b) for Pd(100). The tilted angle was defined as the angle between the axial direction of the dsDNA and the tangential direction of the Pd surface.

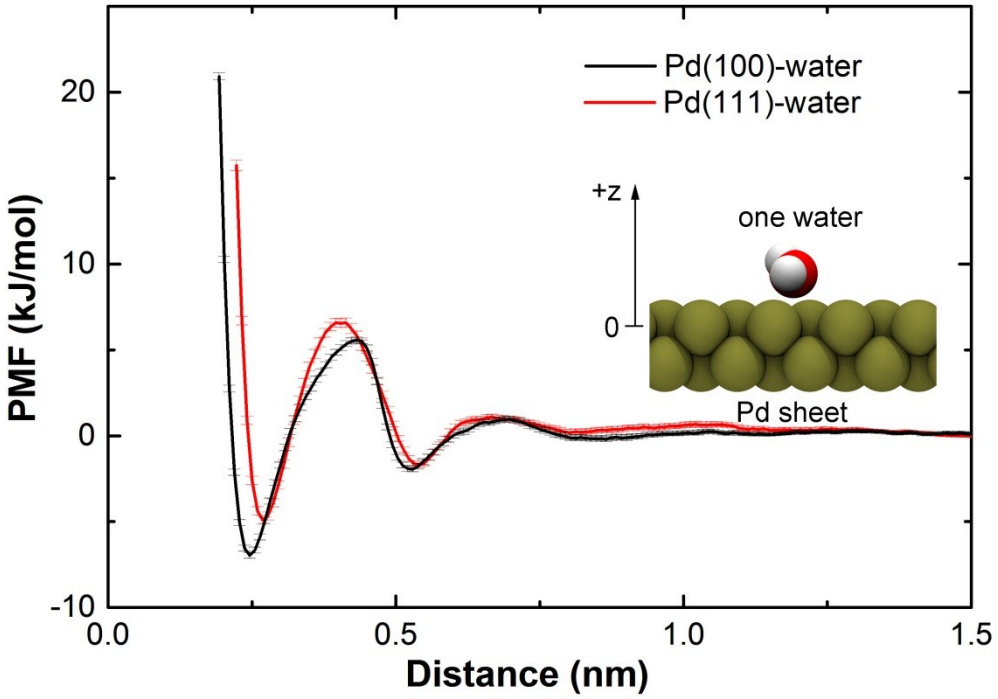

Figure S4. Potential of mean force (PMF) of a water molecule moving along the z-direction of Pd(100) (black curve) and Pd(111) (red curve).

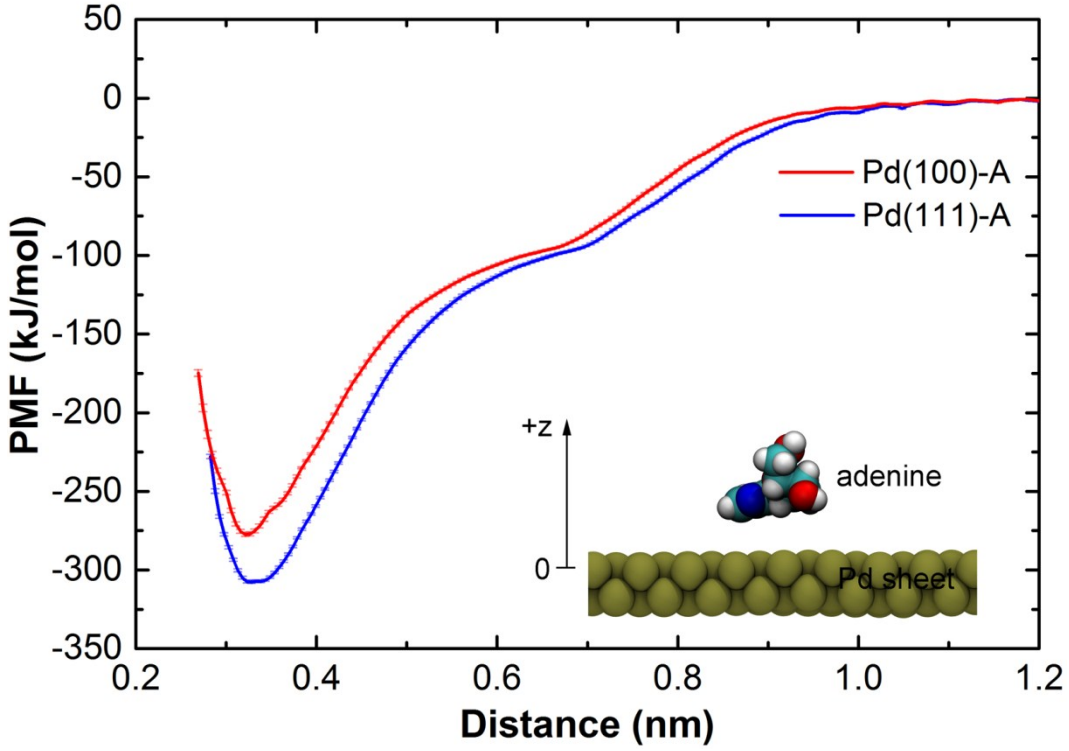

Figure S5. Potential of mean force (PMF) of a deoxyadenosine moving along the z-direction of Pd(100) (red curve) and Pd(111) (blue curve) in gaseous phase environment. The PMF values at two potential wells were -277.2 kJ/mol and -307.2kJ/mol, respectively.

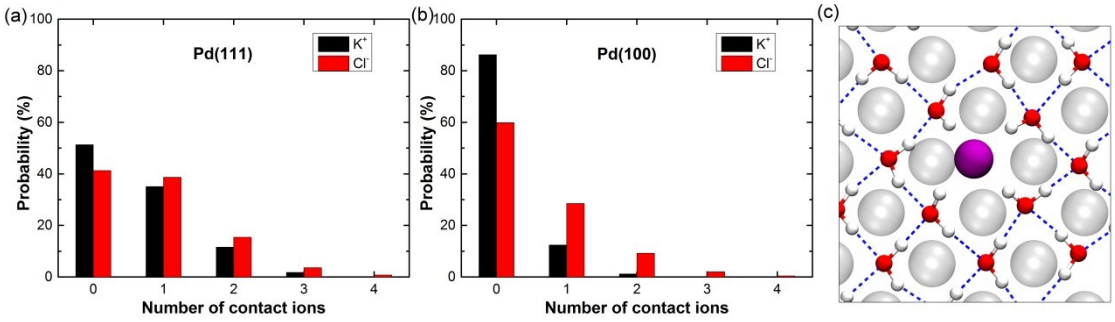

Figure S6. Binding of ions to the two Pd facets. (a-b) The probabilities of direct binding numbers of K^+ and Cl^- to the Pd(111) and Pd(100). (c) The binding configuration of Cl^- to Pd(100) facet. The Pd atoms were shown with transparent spheres, while the Cl^- ion was displayed with a purple sphere. The ball-and-stick models (colored in red and white) were water molecules. The blue dashed lines were hydrogen bonds.