Reaction Mechanism of the Metal Precursor Pulse in Plasma-Enhanced Atomic Layer Deposition of Cobalt and the Role of Surface Facet

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Table S1. The calculated reaction energy for hydrogen transfer step and reaction barriers on Co (001) and (100) surfaces with NH_x terminations corresponding to zero K condition. $E_{adsorption}$ is the energy change upon precursor adsorption, $E_{hydrogen}^{I}$ and $E_{hydrogen}^{II}$ are the energy change for the first and second hydrogen transfer, and $E^{Des}{}_{CpH}^{I}$ is the desorption energy of CpH.

	$H^* + CoCp_2 \rightarrow CoCp^* + HCp$			$H^* + CoCp \rightarrow Co^* + HCp$		
	$E_{adsorption}$	$E_{hydrogen}^{I}$	$E_{barrier}$	$E^{Des}{}_{CpH}^{I}$	$E_{hydrogen}^{II}$	$E_{barrier}$
Co(001)	-0.10	-0.76	1.00	-2.34	-2.46	1.24
Co(100)	-1.73	-3.12	1.56	-1.17	-1.72	0.84

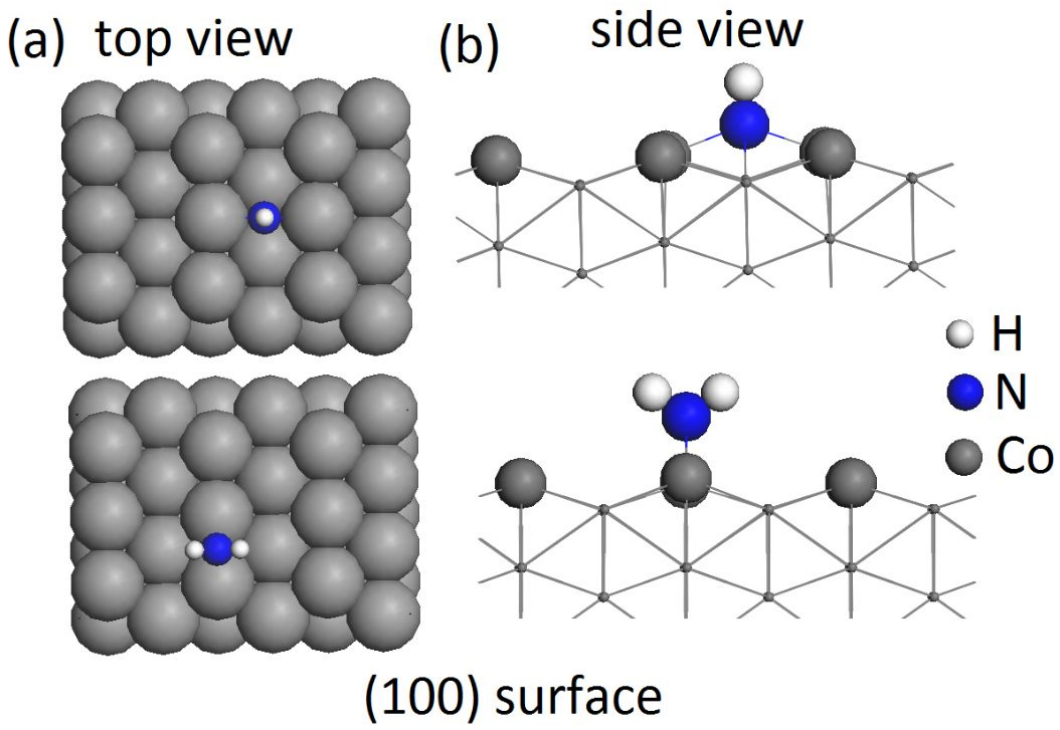

Figure S1. The configurations of the (a) top view and (b) side view of single NH and NH_2 adsorbed on Co(100) surface. NH prefers channel bridge and NH_2 prefers surface bridge site.

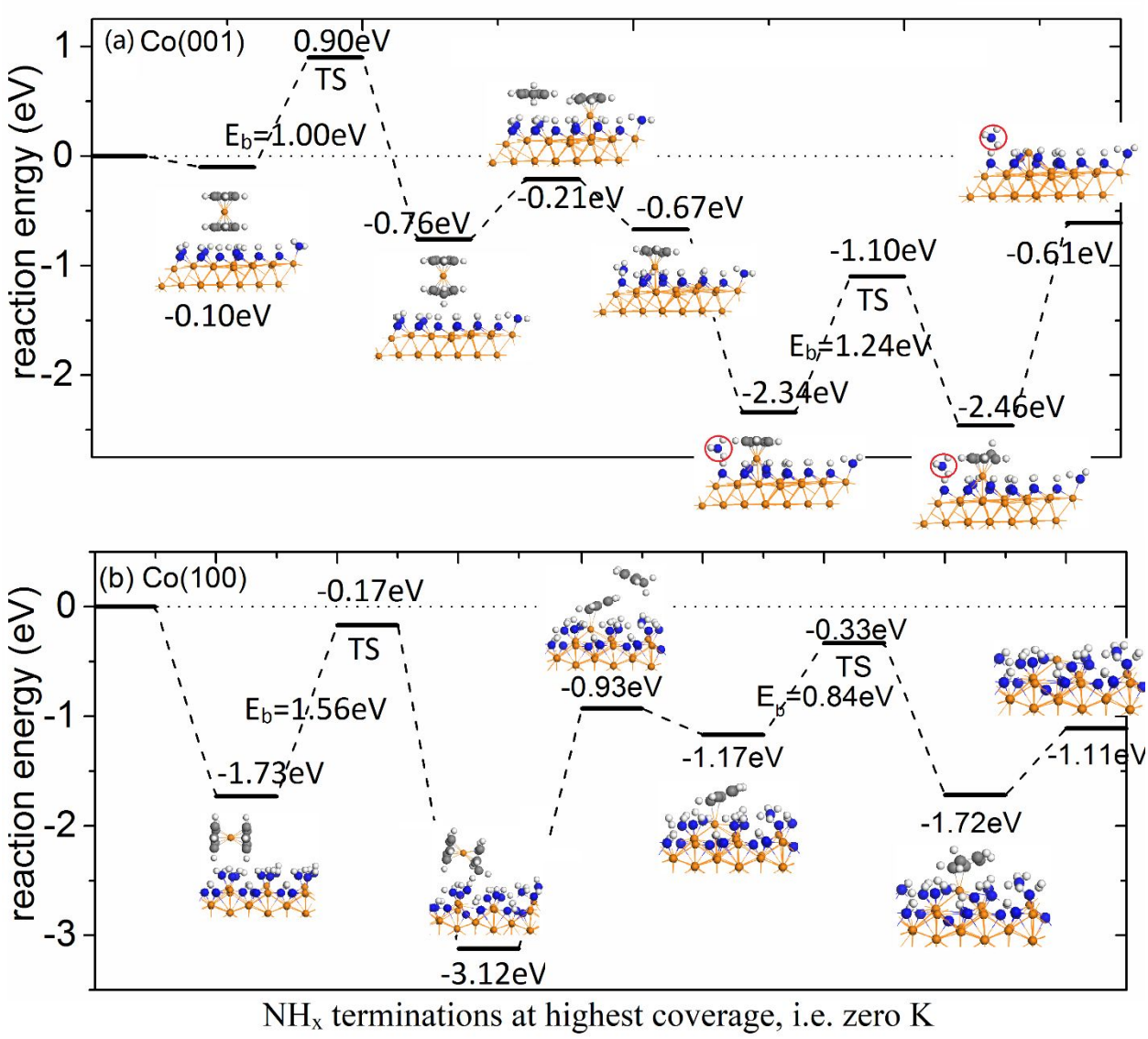

Figure S2. The plotted metal precursor reaction pathway on (a) Co(001) surface and (b) Co(100) surface with NH_x terminations at zero K condition. The Cp ligand is eliminated via hydrogen transfer. The Co atom is represented by orange color and carbon, nitrogen and hydrogen atoms are represented by grey, blue and white color, respectively. On Co(001) surface, there is NH_3 formation during the Cp ligand elimination process.