Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information

An experimental and theoretical study of adenine adsorption on Au(111)

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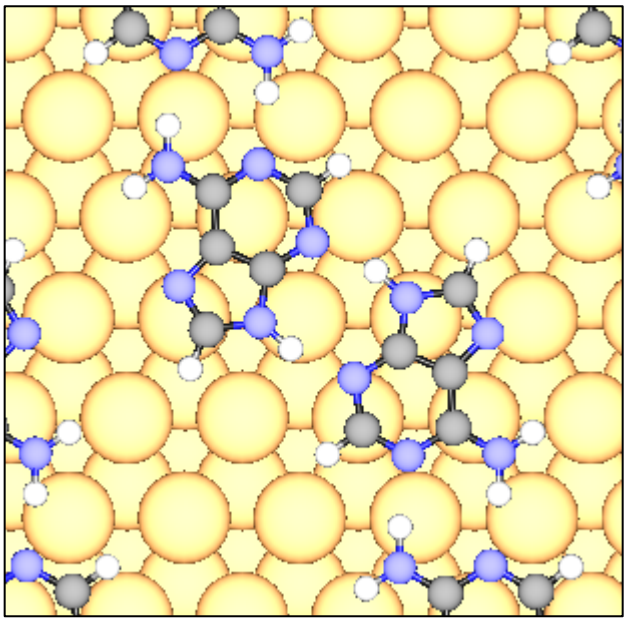

Fig. S1 Top view of optB86b-vdW minimum-energy adsorption mode for a hydrogen-bonded parallel chain structure of N9H adenine on Au(111). Gold, white, black, and blue spheres represent Au, H, C and N atoms, respectively.

Table S1 Nearest H-Au and N-Au distances (dH and dN, in Å) for adenine adsorbed in various upright modes on Au(111)[a]

	RPBE, 500 eV				optB86b-vdW, 500 eV			
	dH1	dH2	dN1	dN2	dH1	dH2	dN1	dN2
N9H (N1)	2.59	2.44	2.64	-	2.44	2.30	2.46	-
N9H (N3)	2.63	2.91	2.68	-	2.22	2.49	2.30	-
N9H (N3) with N9H dissociated	3.18	3.48	2.28	2.21	3.00	3.31	2.21	2.16
N9H (N7)	2.57	2.80	2.83	-	2.42	2.64	2.63	-
N3H (N9)	2.36	2.80	2.31	-	2.25	2.67	2.22	-
N7H (N3,N9)	3.53	3.58	2.65	2.84	3.26	3.28	2.39	2.52

[a] Labels are as indicated in Figure S2. 500 eV denote the cutoff energy used in the DFT calculations; see the Computational Methods for detail.

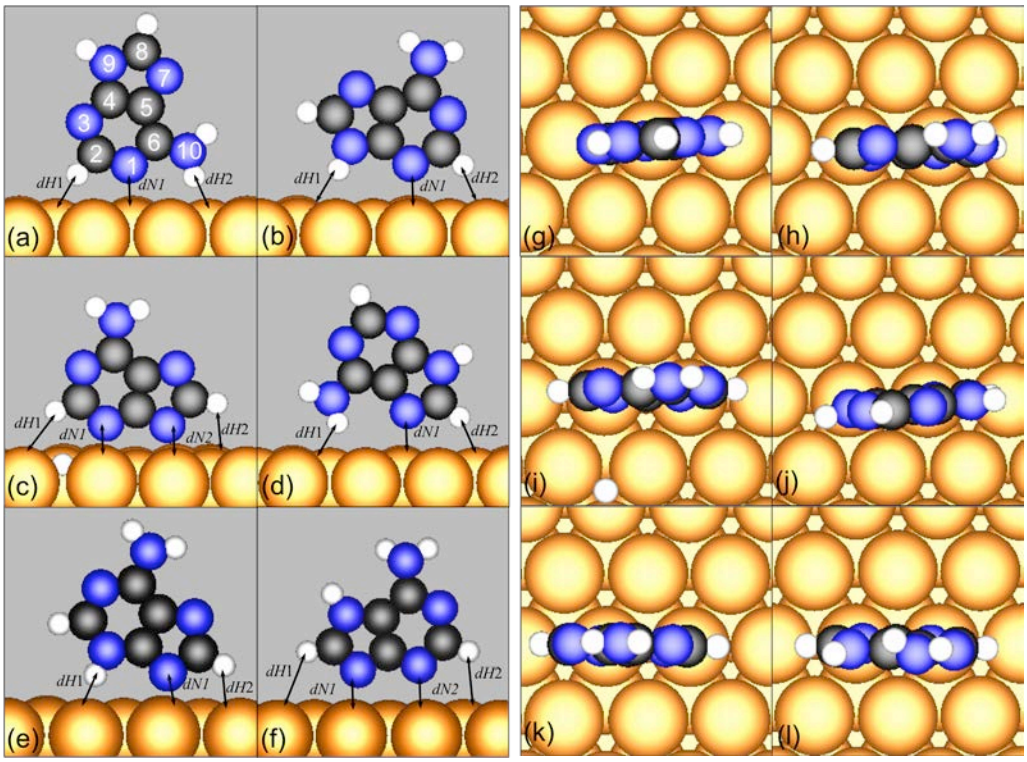

Fig. S2 OptB86b-vdW minimum-energy geometries for (a, g) N9H (N1); (b, h) N9H (N3); (c, i) N9H (N3) with H dissociated; (d, j) N9H (N7); (e, k) N3H (N9) and (f, l) N7H (N3,N9) on Au(111). Left panels show side views and right panels show top views. Gold, white, black and blue spheres represent Au, H, C and N atoms, respectively. For clarity, periodic images of the adsorbates have been removed.