Supplementary Material

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1. Adsorption energy of benzene on Pt(355) and Pt(322) surfaces calculated with the PBE functional

Table S1. The adsorption energies (eV) of C_6H_6 on Pt(355) and Pt(322) surfaces. The results presented here were calculated by using the PBE functional without vdW corrections.

Adsorption sites	Pt(355)	Pt(322)
bridgeA_0°	-0.61	-0.71
bridgeB_0°	-0.63	-0.69
bridgeC_0°	-1.49*	-1.76*
bridgeA_30°	-1.04	-1.16
bridgeB_30°	-1.12	-1.20
bridgeC_30°	-1.36	-1.45
hcpA_0°	-0.48	-0.84
hcpB_0°	-0.61	-0.85
hcpC_0°	-1.01	-1.76
hcpA_30°	-0.83*	-1.12*
hcpB_30°	-1.04*	-1.05*
hcpC_30°	-1.12*	-1.67*
fccA_0°	-0.56	-0.82
fccB_0°	-0.67	-0.74
fccC_0°	-1.49	-1.19
fccA_30°	-0.83*	-1.16*
fccB_30°	-0.90*	-1.20*
fccC_30°	-1.36*	-1.68*
stepA_0°	-1.46*	-0.14
stepA_30°	0.67	-1.42*
stepB_0°	-1.60	-1.10
stepB_30°	-1.46*	-1.23*

*unstable site

2. Core-level binding energy shift of C 1*s* in adsorbed benzene

Table S2. The core level binding energy shift (E_{CLS} in unit of eV) of C 1*s* in benzene on the most stable adsorption sites for Pt(355) and Pt(322) surfaces. The associated numbered carbons are shown in Figure 8. These results are calculated using the PBE functional without vdW corrections.

carbon	Pt(355)	Pt(322)
1	0.32	0.06
2	0.19	0.03
3	0.19	0.03
4	0.33	0.06
5	0.41	0.15
6	0.41	0.15

Table S3. The core level binding energy difference (with respect to C1) of C 1*s* in benzene on the terrace bridgeA_30° sites for Pt(355) and Pt(322) surfaces. The associated numbered carbons are shown in Figure 11a. These results are calculated using the PBE functional with vdW corrections.

carbon	Pt(355)	Pt(322)
1	0.00	0.00
2	0.13	0.15
3	0.01	0.00
4	0.02	0.03
5	0.10	0.10
6	0.03	0.03