

Supporting Information for

Effects of Pd/Pt bimetal supported by γ -Al₂O₃ Surface on Methane Activation

Meiling Hou¹, Xin Zhang¹, Chao Fu¹, Wanglai Cen², Jiaxing Chen^{*1,3}

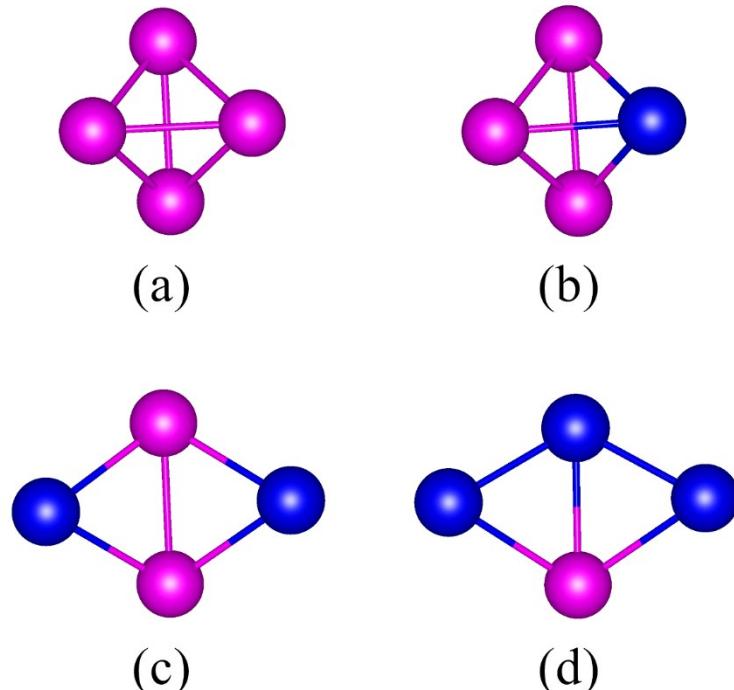


Figure S1. Top view of (4-n)Pd-nPt clusters

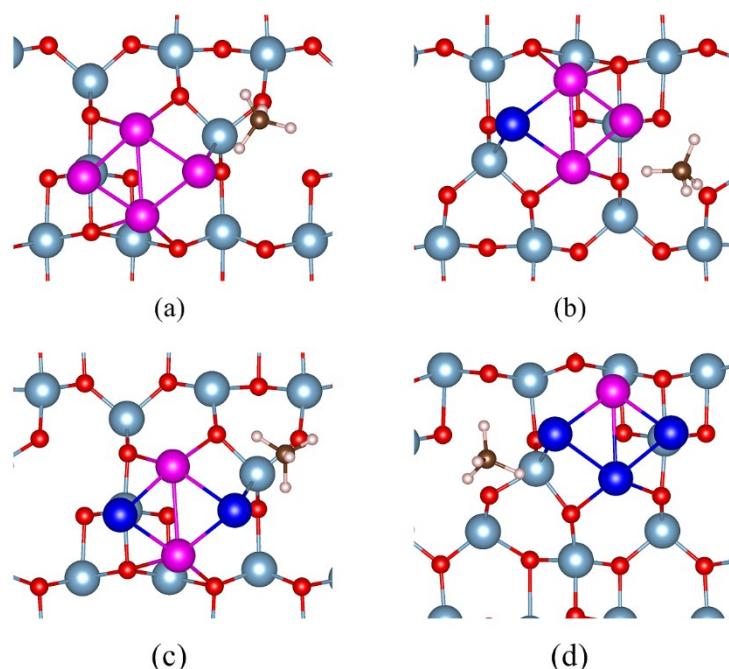


Figure S2. Top view of CH₄ adsorption on (4-n)Pd-nPt/ γ -Al₂O₃

Table S1 The distance of most stable adsorption configurations of (4-n)Pd-nPt clusters on the γ -Al₂O₃ surface.(Å)

	4Pd	3Pd-Pt	2Pd-2Pt	Pd-3Pt
\bar{d} (Pd-Pd)	2.76	2.61	2.86	—
\bar{d} (Pd-Pt)	—	2.91	2.52	2.63
\bar{d} (Pt-Pt)	—	—	3.65	2.52
$d(\text{Pd}_1\text{-O}_3)$	2.26	2.22	2.23	2.20
$d(\text{Pd}_1\text{-O}_4)$	2.15	2.16	2.12	2.13
$d(\text{Pd}_2\text{-O}_1)$	2.16	2.13	2.13	—
$d(\text{Pd}_2\text{-O}_2)$	2.04	2.05	2.03	—
$d(\text{Pd}_3\text{-Al}_A)$	2.59	2.57	—	—
$d(\text{Pd}_4\text{-Al}_B)$	2.47	—	—	—
$d(\text{Pt}_1\text{-Al}_B)$	—	2.44	2.44	2.42
$d(\text{Pt}_2\text{-Al}_A)$	—	—	2.51	2.52
$d(\text{Pt}_3\text{-O}_2)$	—	—	—	2.13
$d(\text{Pt}_3\text{-O}_1)$	—	—	—	2.06
Δq	-0.22	-0.29	-0.34	-0.35

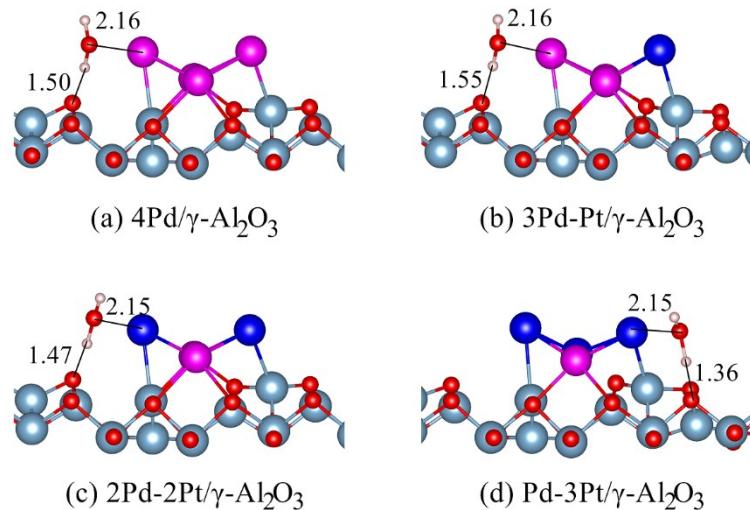


Figure S3 Relaxed adsorption configuration of H₂O on (4-n)Pd-nPt/γ-Al₂O₃ surfaces. (a) 4Pd/γ-Al₂O₃; (b) 3Pd-Pt/γ-Al₂O₃; (c) 2Pd-2Pt/γ-Al₂O₃; (d) Pd-3Pt/γ-Al₂O₃

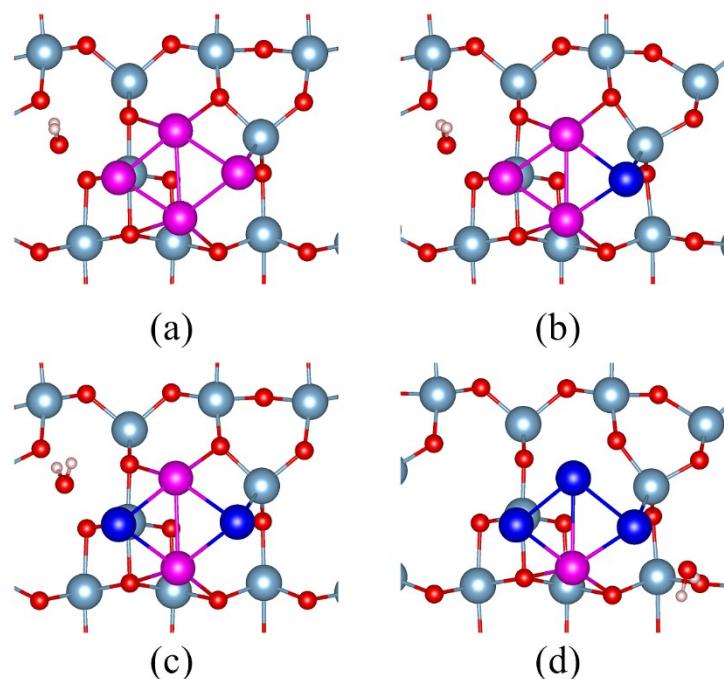


Figure S4. Top view of H₂O adsorption on (4-n)Pd-nPt/γ-Al₂O₃

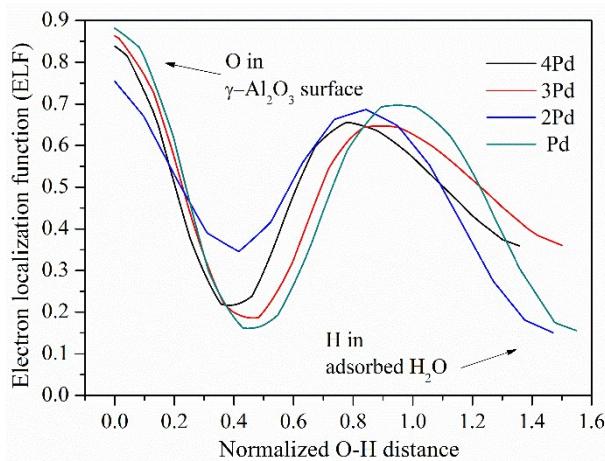


Figure S5 Electron localization function (ELF) between O in $\gamma\text{-Al}_2\text{O}_3$ surface and H in adsorbed H_2O .