

Supplementary data 3.

Table 1s: The calculated Löwdin charge (Δq) referred to the charge of isolated atom:

	N	M	M2	O(-N)	O next to M	Ti next to N	Ti next to M
N _{int} -TiO ₂	-0.26			-0.27		1.59	
N _{subs} -TiO ₂	-0.76						
Pd@TiO ₂		0.28			-0.67		1.53
Pt@TiO ₂		-0.29			-0.53		1.63
Pd ₂ @TiO ₂		0.23	0.24		-0.87		1.50
Pt ₂ @TiO ₂		-0.34	-0.24		-0.56		1.56
Pd@N _{int} -TiO ₂	-0.37	0.38		-0.35	-0.72	1.59	1.59
Pd ^{next} @N _{int} -TiO ₂	-0.25	0.32		-0.26	-0.70	1.59	1.57
Pt@N _{int} -TiO ₂	-0.19	-0.31		-0.34	-0.58	1.66	1.56
Pd@N _{subs} -TiO ₂	-0.97	0.46			-0.72		
Pt@N _{subs} -TiO ₂	-0.82	-0.30			-0.56		
Pd ₂ @N _{int} -TiO ₂	-0.35	0.35	0.26	-0.33	-0.50	1.64	1.62
Pt ₂ @N _{int} -TiO ₂	-0.19	-0.26	-0.4	-0.33	-0.73	1.67	1.63