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Mechanism of a self-assembled Pd (ferrocenylimine)–Si compound-catalysed Suzuki coupling reaction

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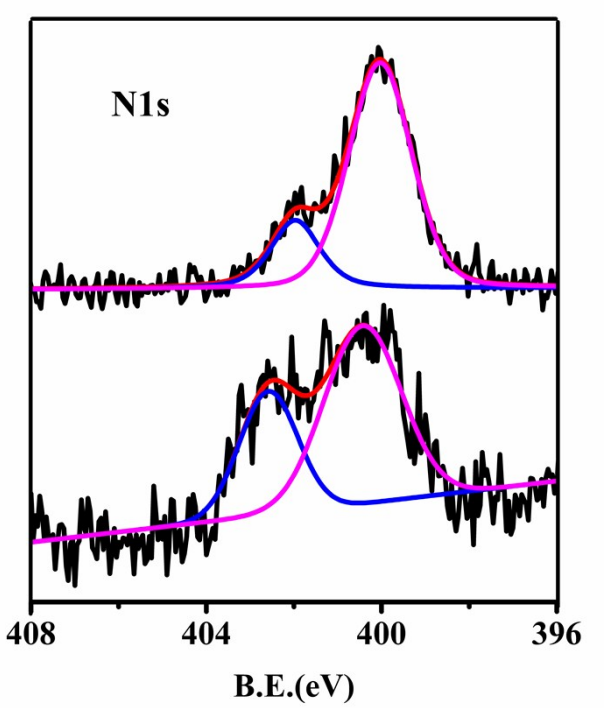


Fig.S1. N1s XPS spectrum of the SAM ferrocenylimine ligand (FcL-Si, curve a) and Pd-ferrocenylimine complex (Pd(FcL)–Si, curve b) on silicon.

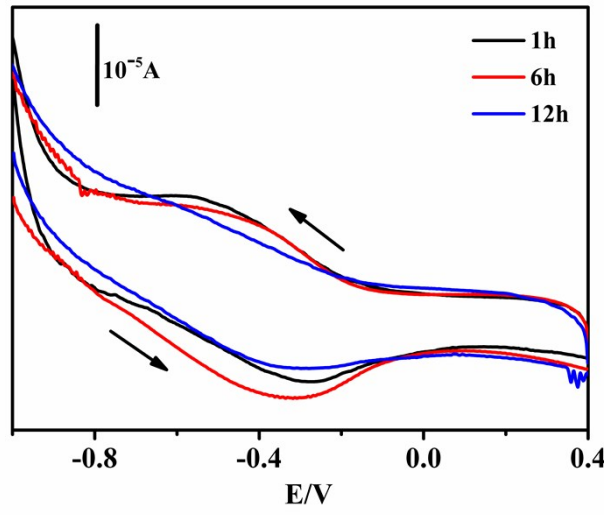


Fig. S2. Cyclic voltammograms of the catalyat-modified ITO at different reaction times in 0.1M N_2-saturated Tris-HCl.

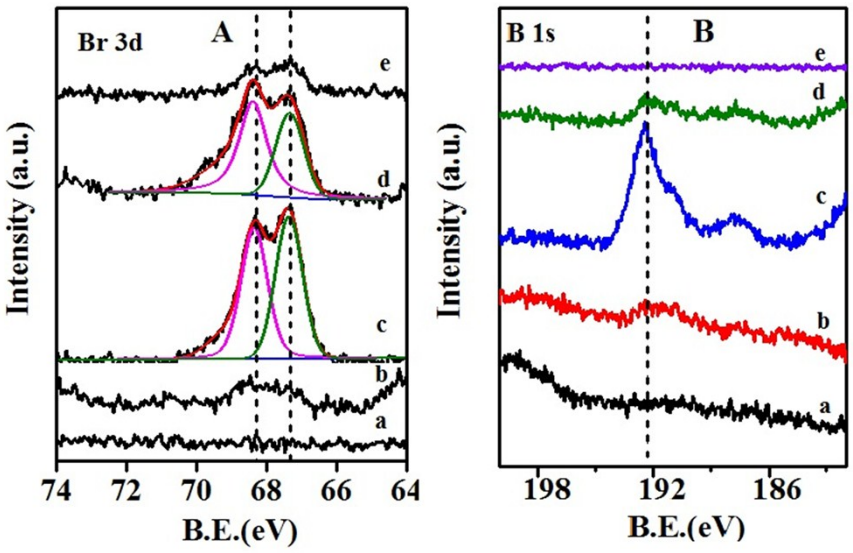


Fig.S3. XPS spectras of Br 3d (A) and B 1s (B) spin orbit doublet of catalytic film at different reaction time. (a) 1 h, (b) 3 h, (c) 6 h, (d) 9 h, (e) 12 h.

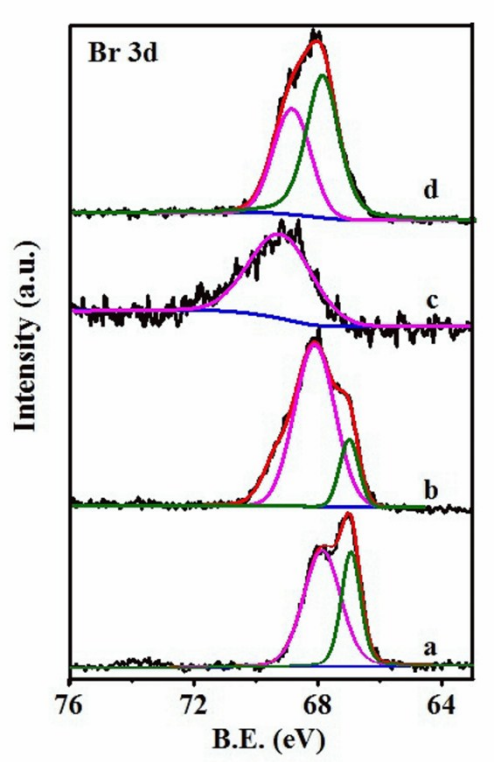
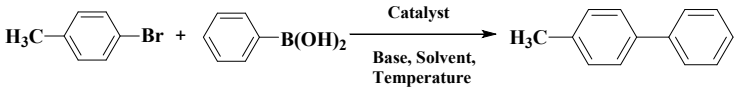


Fig.S4. XPS spectras of Br spin orbit doublet of catalytic film at differenta queous solutions containing (a) K_2CO_3, (b) K_2CO_3+TBAB, (c) K_2CO_3+PhBr, (d) K_2CO_3+TBAB+PhBr.

Table S1 Effect of solvents, bases and temperature on Suzuki cross-reaction. [a]



Entry	Solvent	Base	Time(h)	Temperature (ºC)	Yield[c](%)
1	DMF	K_2CO_3	12	80	5
2	toluene	K_2CO_3	12	80	43
3	DMSO	K_2CO_3	12	80	0
4	Et_3N	K_2CO_3	12	80	0
5	THF	K_2CO_3	12	80	8
6	CH_3OH	K_2CO_3	12	80	48
7	CH_3OH-H_2O(1:1)	K_2CO_3	12	80	50
8	H_2O	Na_2CO_3	12	80	81
9	H_2O	$NaHCO_3$	12	80	69
10	H_2O	NaOH	12	80	64
11	H_2O	NaOAc	12	80	40
12	H_2O	Na_2HPO_4	12	80	32
13	H_2O	KH_2PO_4	12	80	72
14	H_2O	K_3PO_4	12	80	81
15	H_2O	$CsCO_3$	12	80	85

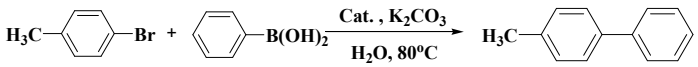
16	H_2O	t-BuNa	12	80	91
17	H_2O	Et_3N	12	80	85
18	H_2O	K_2CO_3	12	40	trace
19	H_2O	K_2CO_3	12	50	37
20	H_2O	K_2CO_3	12	60	54
21	H_2O	K_2CO_3	12	70	73
22	H_2O	K_2CO_3	12	80	94
23[c]	H_2O	K_2CO_3	12	80	35
24	H_2O	K_2CO_3	15	80	96
25	H_2O	K_2CO_3	18	80	97

[a] Reaction conditions: 0.125 mmol of 4-bromotoluene, 0.15 mmol of $PhB(OH)_2$, 0.15 mmol of base and catalyst (1.24×10^{-8} mol·cm^{-2} Pd) in 5.0 mL of solvent at 80ºC, 12h. 0. 15 mmol of TBAB as phase transfer catalyst was added in H_2O as a solvent.

[b] HPLC yield.

[c] In the absence of TBAB

Table S2 Recyclability of Pd (FcL)-Si- catalyzed (1 cm×1cm) Suzuki coupling reaction.



Cycles	1 st	2 nd	3rd	4th	5th
Yields (%)	94	90	91	89	90

Reaction conditions: 4-bromotoluene (0.125 mmol), $PhB(OH)_2$ (0.15 mmo), K_2CO_3 (0.15 mmo), TBAB (0.15 mmo), catalyst (1.24×10^{-8} mol·cm^{-2} Pd) and H_2O (5.0 mL); temperature = 80ºC, 12h. Yield determined by HPLC.