

Supplementary Information for:

**Phenylcarbazole-Stabilized Palladium Catalysts for Efficient
Acetylene Hydrochlorination**

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Figure Captions:

Fig S1 Conversion of acetylene over Pd-PCz/SAC catalyst. Reaction conditions: $T = 160\text{ }^{\circ}\text{C}$, $\text{GHSV}(\text{C}_2\text{H}_2) = 120\text{ h}^{-1}$, and $V(\text{HCl}) : V(\text{C}_2\text{H}_2) = 1.25$

Fig S2 XRD surveys of Pd-based/SAC catalysts

Fig S3 TGA and DTG splines of the fresh (a) and used (b) Pd-PCz/SAC catalysts

Fig S4 XPS surveys of Pd-based/SAC catalysts

Fig S5 XPS pattern of relative nitrogen content in the fresh (a) and used (b) Pd-PCz/SAC catalysts

Fig S6 ESP mapped molecular surface along with ESP array of PdCl_2 & PCz-PdCl_2 (a), $\text{PdCl}_2\text{-PCz-C}_2\text{H}_2$ (b), $\text{PdCl}_2\text{-PCz-HCl}$ (c) and $\text{PdCl}_2\text{-PCz-C}_2\text{H}_3\text{Cl}$ (d)

Fig S7 The most favorable adsorption configuration of C_2H_2 , HCl , and VCM with PdCl_2 and $\text{PdCl}_2\text{-PCz}$ catalyst (all the bond distances are presented in \AA)

Table Captions:

Table S1 Performance of Pd-based catalysts for acetylene hydrochlorination

Table S2 Relative contents of palladium species in catalysts

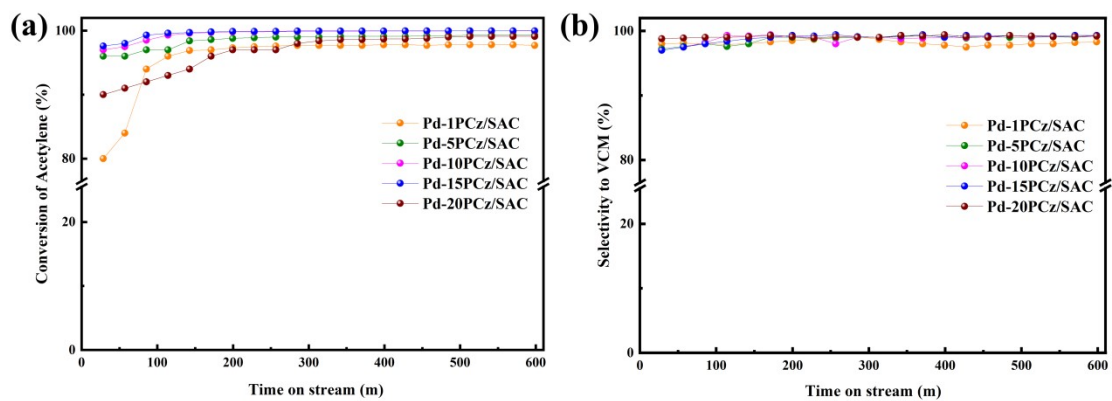


Fig. S1 Conversion of acetylene over Pd-PCz/SAC catalysts. Reaction conditions: $T = 160\text{ }^{\circ}\text{C}$
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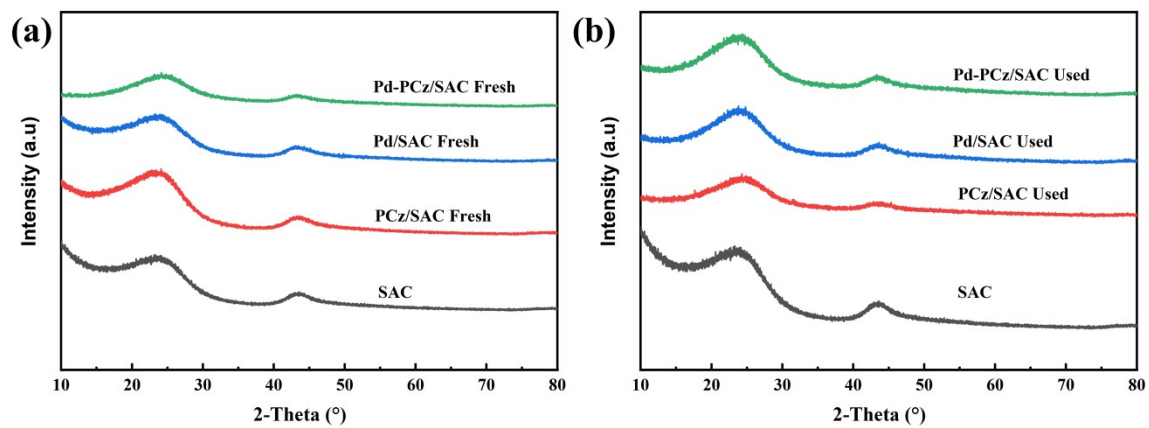


Fig. S2 XRD surveys of Pd-based catalysts

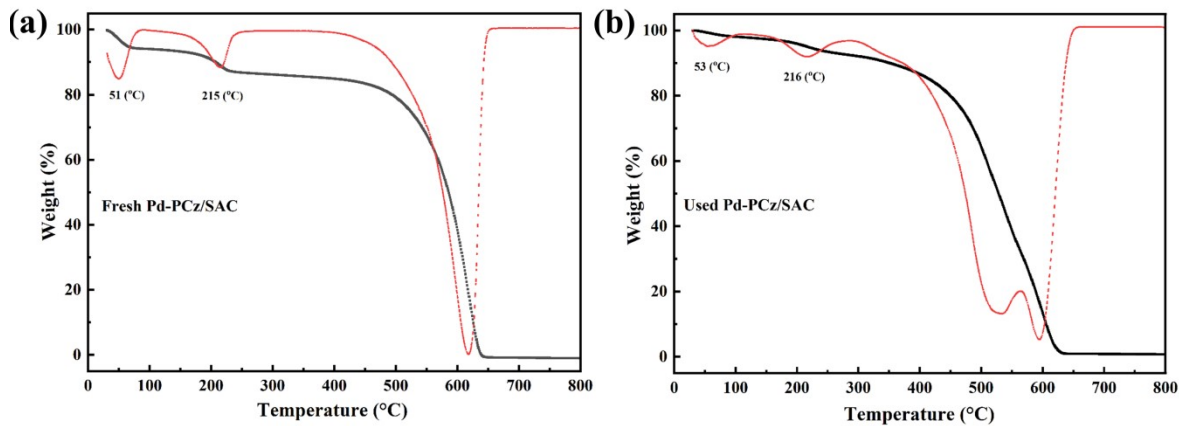


Fig S3 TGA and DTG splines of the fresh (a) and used (b) Pd-PCz/SAC catalysts

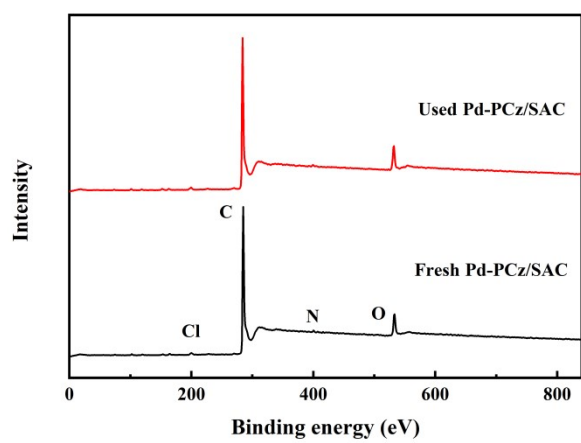


Fig. S4 XPS surveys of Pd-based catalysts

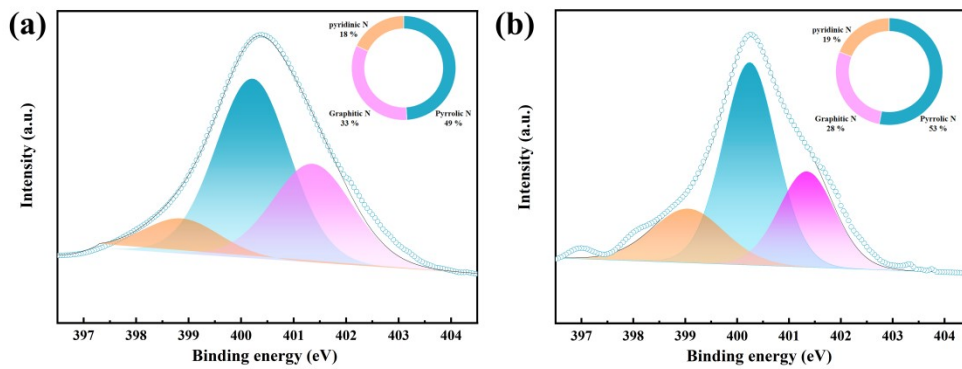


Fig S5 XPS pattern of relative nitrogen content in the fresh (a) and used (b) Pd-PCz/SAC catalysts

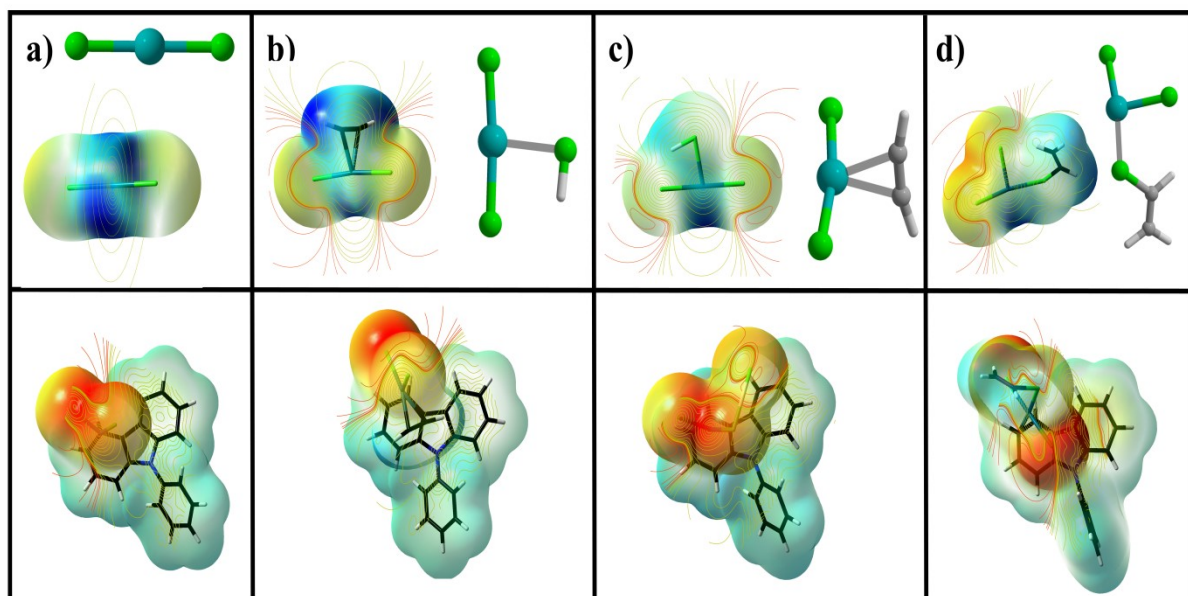


Fig. S6 ESP mapped molecular surface along with ESP array of PdCl₂ & PCz-PdCl₂ (a), PdCl₂-PCz-C₂H₂ (b), PdCl₂-PCz-HCl (c) and PdCl₂-PCz-C₂H₃Cl (d)

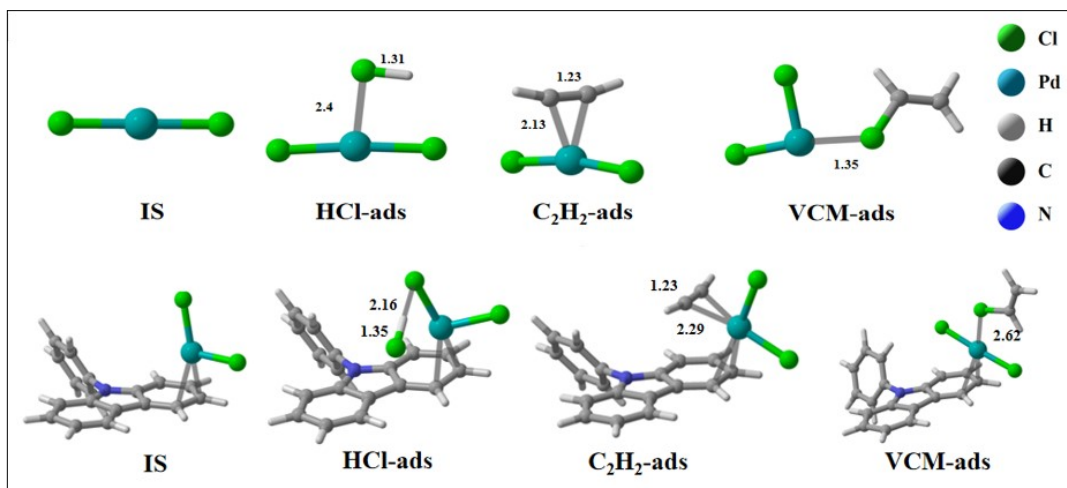


Fig. S7 The most favorable adsorption configuration of C₂H₂, HCl, and VCM with PdCl₂ and PdCl₂-PCz catalyst (all the bond distances are presented in Å)

Table S1 Performance of Pd-based catalysts for acetylene hydrochlorination

Year	Catalyst	GHSV (h ⁻¹)	Temp. (°C)	Acetylene Conversion (%)	Life-time (h)	Ref.
2024	Pd-PCz/SAC	120	160	99	380	This work
2024	Pd-DBF/SAC	120	160	99	400	[1]
2024	Pd@20(4-CB)TPPB/USY	120	160	99.9	52	[2]
2023	Pd-20[DBU][Cl]/AC	360	180	96	24	[3]
2022	Pd@15ChCl@USY	120	160	99	20	[4]
2021	Pd/UHNTs	150	160	90	94	[5]
2020	0.1Pd/NC800-TA	1000	160	94	20	[6]
2020	PANI/CNT-Pd	120	160	91	20	[7]
2019	(NH ₄) ₂ PdCl ₄ /AC	100	100	99	10	[8]
2019	Pd-A-IL/AC	1000	160	91	10	[9]
2019	0.5Pd-10IL/AC	740	160	98	10	[10]
2019	Pd/7B2-HY	110	160	95	30	[11]
2018	PdCl ₂ /NGCS900	79.2	100	90	20	[12]
2018	Pd NPs@[P ₄₄₄₄][C ₁₇ COO]-C ₁₄	41	180	98	72	[13]
2016	Pd/NH ₄ F-urea-HY	120	160	98	8	[14]
2016	Pd/PANI-HY	110	160	95	300	[15]
2016	Pd-K/NFY	110	160	99	50	[16]
2015	Pd-K/HY	110	160	95	2	[17]
2013	Pd/HY	110	160	95	1	[18]
2010	PdCl ₂ /C	120	160	98	3	[19]

Table S2 Relative content of Pd species in the fresh and used catalysts

Catalysts	Pd ²⁺	Pd ⁰
Fresh Pd/SAC	63	37
Used Pd/SAC	58	42
Fresh Pd-PCz/SAC	68	32
Used Pd-PCz/SAC	65	35

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