

Electronic Supplementary Material

Structural insight into palladium-nickel clusters over mordenite zeolite for carbene-insertion reaction

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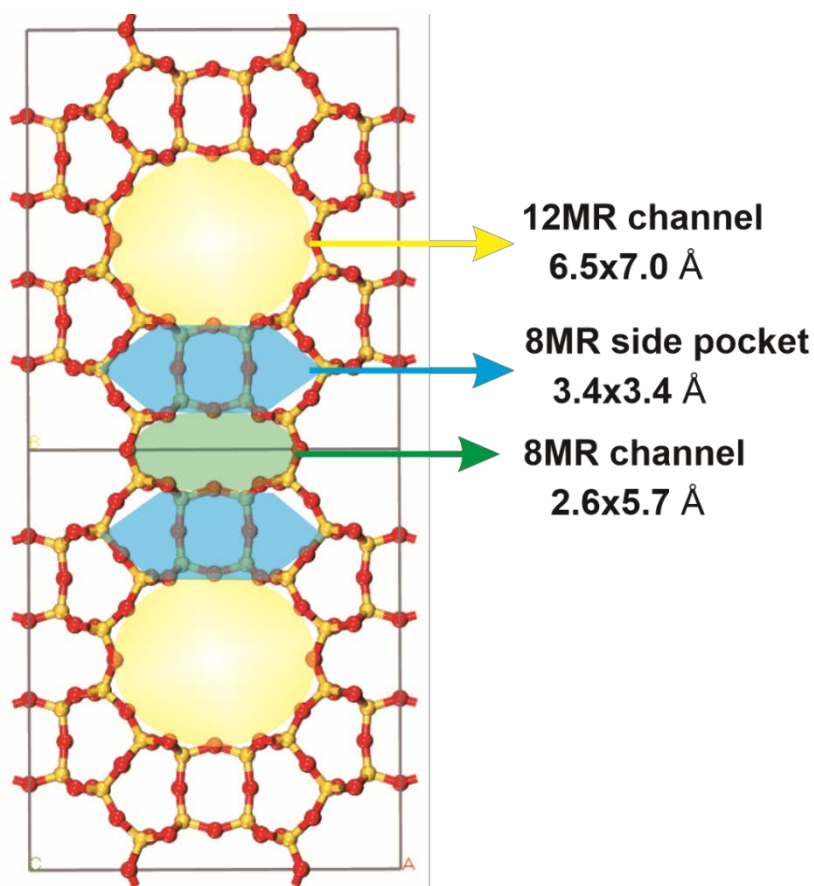


Figure S1. Structure and pore sizes of MOR zeolite.

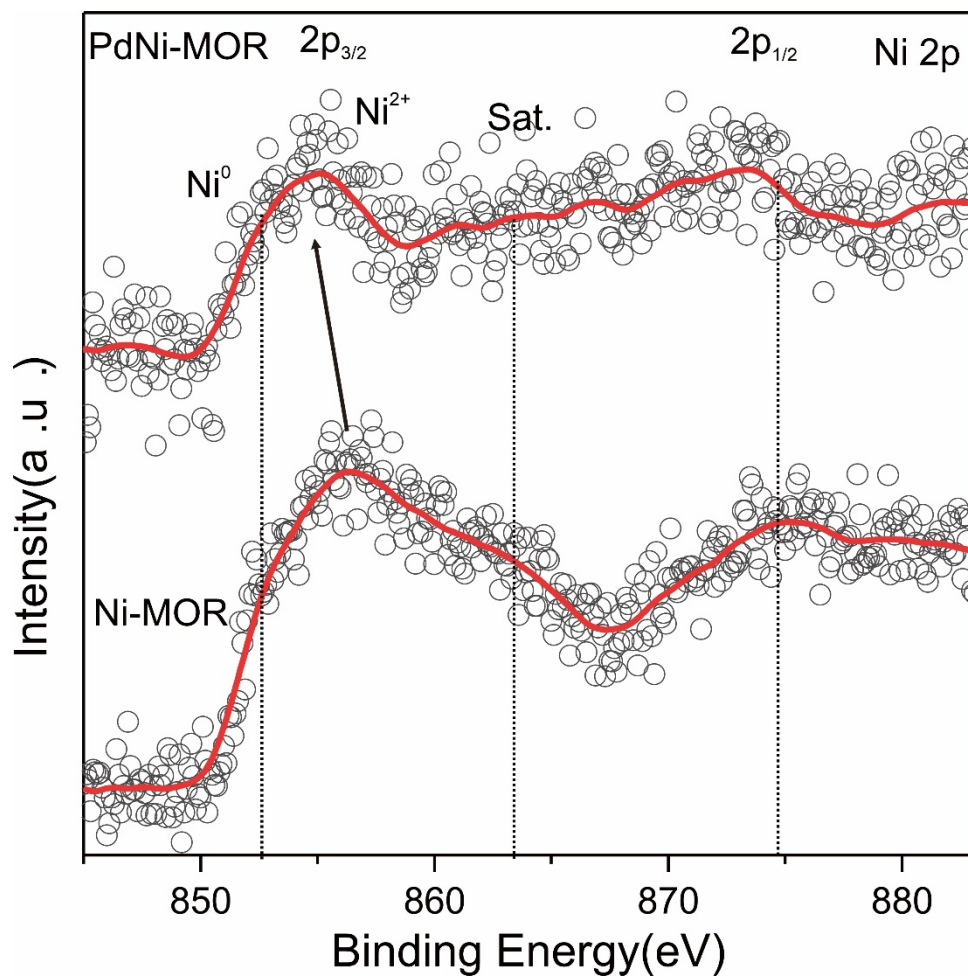


Figure S2. Ni 2p XPS spectrum of the Ni-MOR and PdNi-MOR samples.

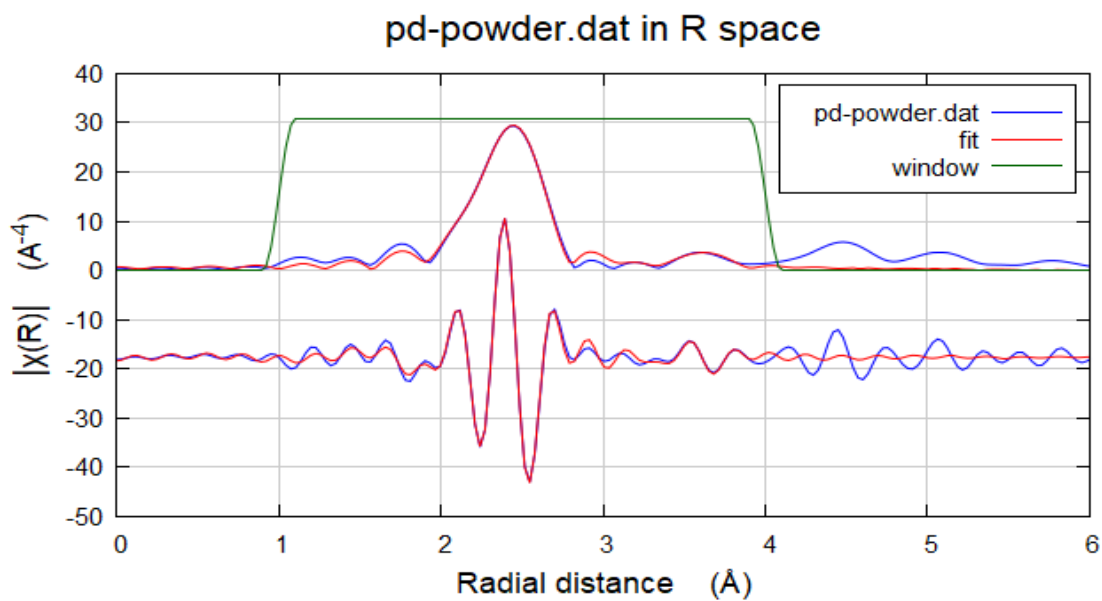


Figure S3. EXAFS fitting of Pd foil with k₂-weighted q-space with R-range at 0.9-4.1 Å.

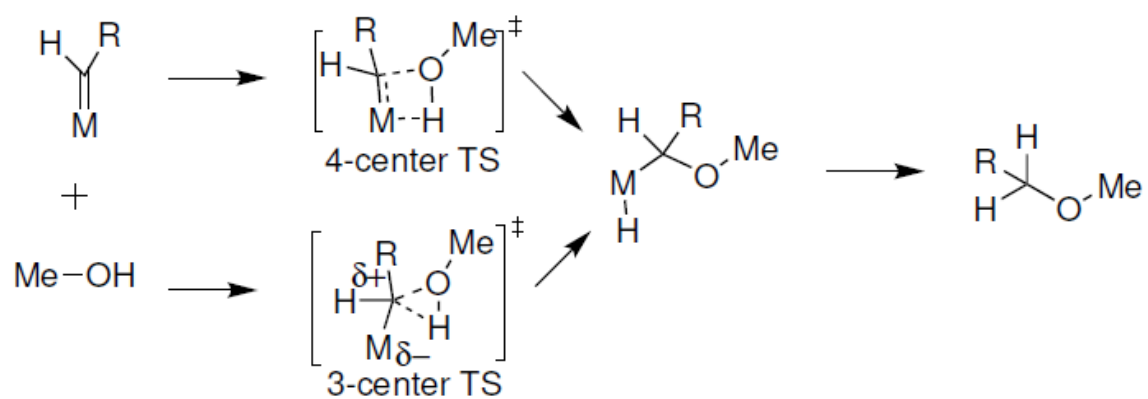


Figure S4. Common insertion mechanism through either a 3 or 4-centered transition state. [J. Am. Chem. Soc. 2002, 124, 24, 7181–7192]

Table S1. Crystallographic data and details of pristine MOR, PdNi-MOR based on SXRD

Samples	pristine MOR	PdNi-MOR
Crystal system	Orthorhombic	Orthorhombic
Space group	Cmcm	Cmcm
2 θ range refinement	2 – 80 °	2 – 80 °
Detector	MYTHEN 2D plate detector	MYTHEN 2D plate detector
Refinement methods	Rietveld	Rietveld
a (Å)	18.09 (5)	18.10 (2)
b (Å)	20.25 (6)	20.38 (7)
c (Å)	7.46 (9)	7.50 (2)
V (Å ³)	2737.93 (33)	2769.00 (94)
Rwp / Rp / Rexp (%)	6.4/4.40.79	9.4/6.3/0.83
Wavelength (Å)	0.6895561	0.6895561
2 θ Zero point (°)	-0.00015	0.00015
Gof χ^2	8.03	11.27

Table S2. Crystallographic information files from the Rietveld refinement of pristine MOR based on SXRD.

Species	Atom	X	Y	z	SOF	Beq (Å ²)
Zeolite framework	O1	0.2776(5)	0.0000	0.0000	1	4.8218(2)
	O2	0.3337(8)	0.0819(3)	0.2184(5)	1	4.8218(2)
	O3	0.3754(6)	0.0884(6)	0.9417(2)	1	4.8218(2)
	O4	0.2392(9)	0.1218(8)	1.0070(5)	1	4.8218(2)
	O5	0.3428(1)	0.3083(1)	0.1507(5)	1	4.8218(2)
	O6	0.25	0.25	0.0028(3)	1	4.8218(2)
	O7	0.3680(1)	0.3126(9)	0.9304(8)	1	4.8218(2)
	O8	0.0000(0)	0.4129(3)	0.2500	1	4.8218(2)
	O9	0.0971(2)	0.3070(7)	0.2500	1	4.8218(2)
	O10	0.0000	0.1926(8)	0.2500	1	4.8218(2)
	Si1	0.3067(4)	0.0753(9)	0.0327(2)	1	0.0991(7)
	Si2	0.3011(7)	0.3154(1)	0.0380(4)	1	0.0991(7)
	Si3	0.0931(3)	0.3817(7)	0.2500	1	0.0991(7)
	Si4	0.0847(1)	0.2251(6)	0.2500	1	0.0991(7)

Table S3. Crystallographic information files from the Rietveld refinement of PdNi-MOR based on SXR. D.

Species	Atom	X	Y	z	SOF	Beq (Å ²)
Zeolite framework	O1	0.2677(5)	0.0000	0.0000	1	3.9803(1)
	O2	0.3260(9)	0.0807(2)	0.2500	1	3.9803(1)
	O3	0.3724(6)	0.0903(5)	0.9778(1)	1	3.9803(1)
	O4	0.2330(6)	0.1171(9)	1.0004(1)	1	3.9803(1)
	O5	0.3567(2)	0.2935(8)	0.2500	1	3.9803(1)
	O6	0.2500	0.2500	0.0000	1	3.9803(1)
	O7	0.3565(5)	0.2971(7)	0.9409(1)	1	3.9803(1)
	O8	0.0000	0.3941(8)	0.2500	1	3.9803(1)
	O9	0.0883(9)	0.3069(4)	0.2500	1	3.9803(1)
	O10	0.0000	0.1752(8)	0.2500	1	3.9803(1)
	Si1	0.2992(5)	0.0725(6)	0.0311(3)	1	3.9803(1)
	Si2	0.3049(3)	0.3125(3)	0.0510(5)	1	3.9803(1)
	Si3	0.0911(2)	0.3777(2)	0.2500	1	3.9803(1)
	Si4	0.0927(7)	0.2319(5)	0.2500	1	3.9803(1)
PdNi Cluster	Pd1	0.4189(1)	0.2263(8)	0.2500	0.376(6)	0.312(2)
	Ni	0.5000	0.1616(7)	0.2500	0.2030(6)	0.312(2)
	Pd2	0.2111(3)	0.45000	0.2500	0.3924(2)	0.312(2)