Supplementary Information

The Effect of Gamma-Al_2O_3 Support on the NO Adsorption on Pd_4 Cluster

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Table S1. Absolute energy (a.u.) and expectation value of the total spin after annihilation of the first spin contaminant (<S^2>**)** for different electronic spin states of $Pd_4/Al_{14}H_6O_{24}$

Electronic spin state	$Pd_4/Al_{14}H_6O_{24}$	
	E / a.u.	<S^2>
1	–2345.50559	7.39
3	–2345.52190	2.29
5	–2345.52197	6.00
7	–2345.50820	12.00

E: absolute energy; <S^2>: expectation value of the total spin after annihilation of the first spin contaminant.

Table S2. BSSE for adsorption energies ($E_{ad.}$, kcal mol^{-1}) of nitric oxide adsorbed on planar and on tetrahedral Pd_4

Form	Pd_4 (planar, D_{2h})				Pd_4 (tetrahedral, Td)		
	Atop (1)(A)	Atop (2)(B)	Bridge(C)	Hollow(D)	Atop(E)	Bridge(F)	Hollow(G)
$E_{ad.}$ / (kcal mol^{-1})	–34.31	–32.42	–43.41	–40.96	–32.64	–31.79	–24.10
$E_{ad.(corr)}$ / (kcal mol^{-1})	–32.68	–30.65	–41.22	–38.01	–30.57	–29.20	–21.02
ΔE / (kcal mol^{-1})	1.63	1.77	2.19	2.95	2.07	2.59	3.08

$E_{ad.}$: adsorption energy; $E_{ad.(corr)}$: corrected adsorption energy; ΔE: energy difference.

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Table S3. BSSE for adsorption energies ($E_{ad.}$, kcal mol^{-1}) of nitric oxide adsorbed on both Pd_4 supported on $Al_{14}O_{24}H_6$ and on the isolated Pd_4 with distorted geometry

	$NO/Pd_4/Al_{14}H_6O_{24}$			$NO/Pd_{4(distorted)}$		
	45	46	47	45	46	47
$E_{ad.}$ / (kcal mol^{-1})	–21.74	–8.79	–28.42	–29.57	–28.10	–34.56
$E_{ad.(corr)}$ / (kcal mol^{-1})	–18.39	–5.80	–25.60	–26.69	–25.45	–31.85
ΔE / (kcal mol^{-1})	3.35	2.99	2.82	2.88	2.65	2.71

$E_{ad.}$: adsorption energy; $E_{ad.(corr)}$: corrected adsorption energy; ΔE: energy difference.