

Supporting Information

Table S1. Calculated Activation Energies (E_a) and Gibbs Free Energies (ΔG) of $\text{NO}_{(a)} \rightarrow \text{N}_{(a)} + \text{O}_{(a)}$ on DI-Rh₁₉ and DI-Ni₁₉ Clusters in Different Temperatures (80K, 250K and 1073K), respectively.

Reaction Paths	$\text{NO}_{(a)} \rightarrow \text{N}_{(a)} + \text{O}_{(a)}$					
	$E_a(80\text{K})$ /eV	$\Delta G(80\text{K})$ / eV	$E_a(250\text{K})$ /eV	$\Delta G(250\text{K})$ / eV	$E_a(1073\text{K})$ /eV	$\Delta G(1073\text{K})$ / eV
DI-Rh ₁₉ -THB(path I)	0.90	-0.80	0.88	-0.80	0.85	-0.77
DI-Rh ₁₉ -BHB(path II)	0.24	-1.63	0.24	-1.62	0.26	-1.58
DI-Ni ₁₉ -THB(path I)	1.00	-1.61	1.00	-1.60	1.02	-1.49
DI-Ni ₁₉ -BHB(path II)	0.41	-1.80	0.40	-1.82	0.38	-1.76