Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information: Highly Effective Catalysis of the Double-icosahedral Ru_{19} Cluster for Dinitrogen Dissociation –A First-Principle Investigation

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TABLE S1. Calculated adsorption energy, bond length, vibrational wavenumbers and total charge population (Δq / |e|) of N_2 on a Ru_{19} cluster.

Site	E_{ads} / eV	d(N-N) / Å	d(Ru-N) / Å	Δq / |e|	ν(N-N) / cm^{-1}
$T_{1(side\text{-}on)}$	-0.81	1.17	2.12	-0.51	1860
$T_{2(side\text{-}on)}$	-0.44	1.17	2.13	-0.45	1865
$T_{3(side\text{-}on)}$	-0.41	1.17	2.12	-0.47	1902
$B_{1(end\text{-}on)}$	-0.82	1.15	2.02	-0.47	2000
$B_{2(end\text{-}on)}$	-0.61	1.15	2.13	-0.46	1951
$B_{3(end\text{-}on)}$[a]	-	-	-	-	-
$H_{1(end\text{-}on)}$[a]	-	-	-	-	-
$H_{2(end\text{-}on)}$[a]	-	-	-	-	-
$H_{3(end\text{-}on)}$[a]	-	-	-	-	-

[a] Adsorption of N_2 at B_3 site by end-on configuration is unstable and eventually shifts to T_2 site. Similarly, adsorption of N_2 at H_1, H_2 and H_3 sites by end-on configuration would also shift to the T_1, T_2 and T_3 sites, respectively.

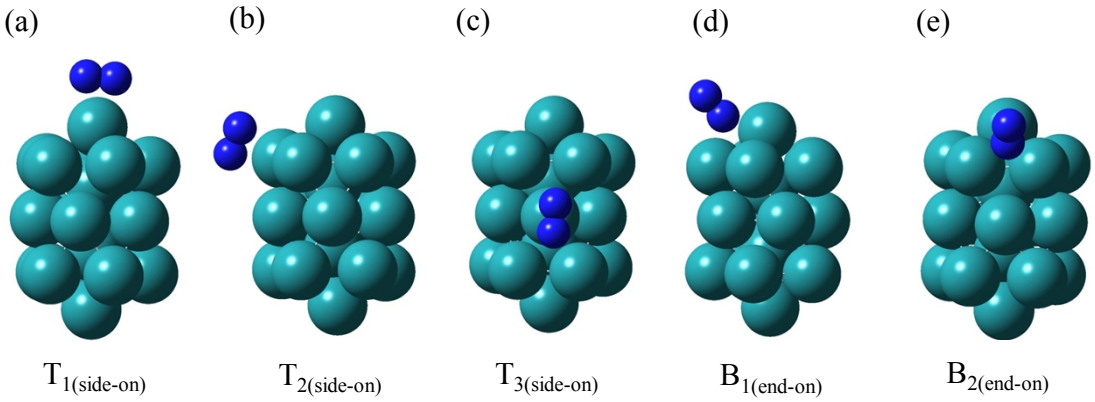

Figure S1. Adsorption geometries of N_2 adsorbed on a DI-Ru_{19} cluster : (a) $T_{1(side\text{-}on)}$, (b) $T_{2(side\text{-}on)}$, (c) $T_{3(side\text{-}on)}$, (d) $B_{1(end\text{-}on)}$ and (e) $B_{2(end\text{-}on)}$.