SUPPLEMENTARY INFORMATION

Density functional theory study of structure, electronic and magnetic properties of non-metal (Group 13) doped stable Rh_n(n=2-8) clusters and their catalytic activities towards methanol activation

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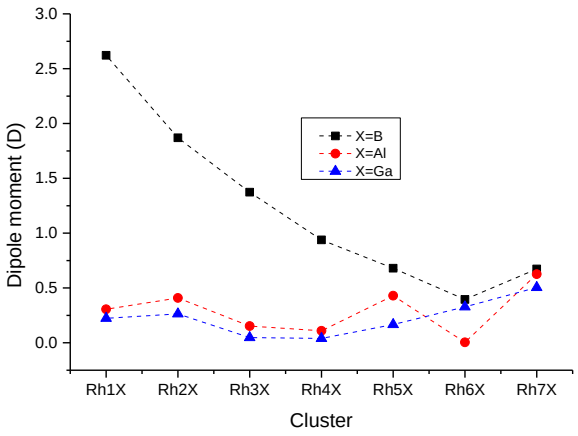
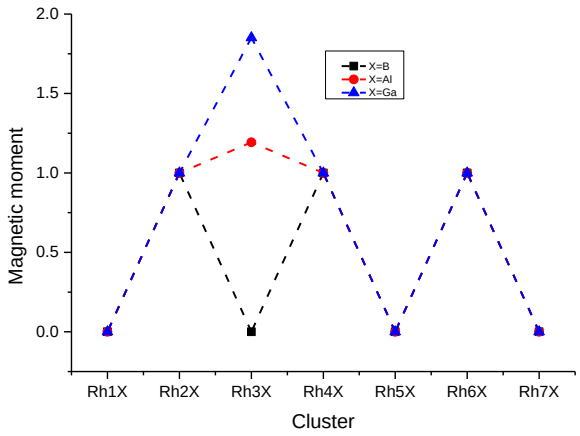
Table S1. BSSE correction of energy (eV) including of DFT derived Rh_nX (n=1-7 and X=B, Al or Ga) clusters

Cluster	(X=B)	(X=Al)	(X=Ga)
Rh_1X	0.08	0.03	0.10
Rh_2X	-0.03	-0.04	-0.03
Rh_3X	0.12	0.07	0.03
Rh_4X	-0.07	-0.06	-0.07
Rh_5X	0.10	0.09	0.08
Rh_6X	-0.07	-0.03	-0.06
Rh_7X	0.09	0.12	0.06



Dipole moment of Rh_nX (n=1-7 and X=B, Al or Ga) clusters



Magnetic moment values of Rh_nX (n=1-7 and X=B, Al or Ga) clusters

Figure S2: Dipole moment and magnetic moments of doped clusters

Table S3: Coordinates of reactants and transition states involved in methanol activation

Rh5_B (Reactant)

Rh	1.21800000	-1.59500000	2.15100000
B	-0.45400000	-0.55500000	2.08500000
Rh	-1.18700000	-2.27600000	1.47800000
Rh	1.37400000	-0.23900000	0.02600000
Rh	-0.62000000	1.04700000	1.01700000
Rh	-0.94700000	-0.89500000	-0.61200000
C	-0.59280886	2.55656340	2.37524211
O	-0.12680886	2.00356340	3.64724211
H	-0.26380886	1.03856340	3.60224211
H	-1.68680886	2.48356340	2.25224211
H	-0.05380886	2.08956340	1.50124211
H	-0.31180886	3.61656340	2.36224211

Rh5_B (Transition state)

Rh	1.21417745	-1.64543639	2.12845896
B	-0.45782255	-0.60543639	2.06245896
Rh	-1.19082255	-2.32643639	1.45545896
Rh	1.37017745	-0.28943639	0.00345896
Rh	-0.62382255	0.99656361	0.99445896
Rh	-0.95082255	-0.94543639	-0.63454104
C	-0.60089933	2.51119174	2.34105129
O	-0.12636349	1.94806229	3.63635085
H	-0.24107716	0.49585822	2.97341818
H	-1.69489933	2.43819174	2.21805129
H	-0.06189933	2.04419174	1.46705129
H	-0.31989933	3.57119174	2.32805129

Rh4_Al (Reactant)

Rh	-3.20283576	0.28636591	0.02615108
Rh	-1.15183576	-1.15763409	0.09215108
Al	-0.20683576	1.00536591	-0.14684892
Rh	-2.12379878	2.52166395	0.20690955
Rh	-1.55583576	0.56536591	1.95115108
O	0.36544878	2.29711816	-0.85689330
C	1.59806396	1.51742701	-1.10817307
H	1.49806396	0.87142701	-1.99517307
H	1.86406396	0.88342701	-0.24717307
H	2.42706396	2.21842701	-1.28517307
H	-0.56612770	2.50665858	-1.11834706

Rh4_Al (Transition state)

Rh	3.20700000	0.28900000	0.02700000
Rh	-1.15600000	-1.15500000	0.09300000
Al	-0.21100000	1.00800000	-0.14600000
Rh	-2.06300000	2.52700000	0.13500000

Rh	-1.56000000	0.56800000	1.95200000
O	0.66066740	2.23241177	-0.77202039
C	1.90161106	1.44745244	-1.02499800
H	1.80161106	0.80145244	-1.91199800
H	2.16761106	0.81345244	-0.16399800
H	2.73061106	2.14845244	-1.20199800
H	-0.93463782	2.57393119	-1.12876366