

Electronic Supplementary Information (ESI)

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Table S1. Average length (Å) values of neutral, cationic and anionic cluster evaluated at BLYP/DNP level.

Cluster size	Neutral	Cationic	Anionic
Rh ₂	2.308	2.355	2.353
Rh ₃	2.448	2.448	2.494
Rh ₄	2.518	2.512	2.550
Rh ₅	2.532	2.538	2.543
Rh ₆	2.491	2.484	2.497
Rh ₇	2.539	2.521	2.527
Rh ₈	2.459	2.474	2.461

Table S2. LUMO-HOMO gap (eV) of Rh_n(n=2-8) clusters calculated at BLYP/DNP level

Cluster size	Neutral cluster	Anionic cluster	Cationic cluster
Rh ₂	0.423	0.161	0.283
Rh ₃	0.604	0.400	0.432
Rh ₄	1.158	0.885	1.006
Rh ₅	0.246	0.262	0.369
Rh ₆	0.365	0.106	0.199
Rh ₇	0.033	0.165	0.213
Rh ₈	0.165	0.064	0.107

Table S3: Vertical ionization energy, electron affinity, chemical hardness, electro negativity and electrophilicity values in eV of Rh_n (n=2-8) clusters


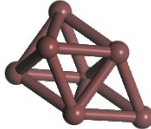
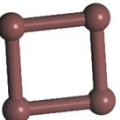

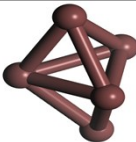
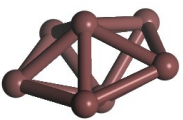

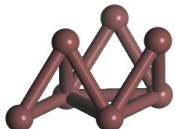
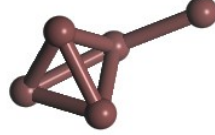
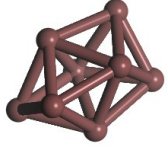
	Vertical ionization energy	Vertical electron affinity	Hardness	Electro negativity	Electrophilicity
Rh ₂	7.503	0.900	3.301	4.201	2.674
Rh ₃	7.033	0.779	3.126	3.906	2.439
Rh ₄	6.480	0.505	2.987	3.492	2.041
Rh ₅	5.905	0.977	2.463	3.441	2.403

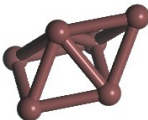
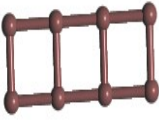
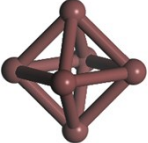
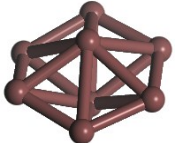
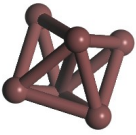


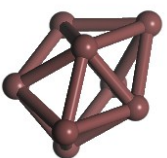

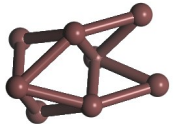
Rh ₆	5.455	1.484	1.985	3.470	3.032
Rh ₇	5.761	1.500	2.130	3.631	3.094
Rh ₈	5.687	1.709	1.989	3.698	3.438

Table S4. Dipole moment (Debye) values of Rh_n (n=2-8) clusters evaluated at BLYP/DNP level.

	Neutral	Cationic	Anionic
Rh ₂	0.0000	14.6898	5.696
Rh ₃	0.0000	7.1021	16.8530
Rh ₄	0.0030	5.8332	5.8328
Rh ₅	0.0765	5.6725	5.6343
Rh ₆	0.0030	9.5131	9.512
Rh ₇	0.1099	6.1883	6.4639
Rh ₈	0.0506	6.1127	6.086

Fig S1. Geometries and point group symmetry of all optimized isomers of Rh_n (n=2-8) cluster.

Cluster size	Point group	Geometry	Cluster size	Point group	Geometry
Rh _{3_2}	C _{2v}		Rh _{7_2}	C _{3v}	
Rh _{4_2}	D _{4h}		Rh _{7_4}	C _s	
Rh _{5_1}	D _{3h}		Rh _{7_5}	D _{5h}	
Rh _{5_3}	C _{4v}		Rh _{7_6}	C _{3v}	
Rh _{5_4}	C ₁		Rh _{8_1}	D _{2d}	

Rh ₆ _1	C _s		Rh ₈ _2	D _{2h}	
Rh ₆ _2	O _h		Rh ₈ _3	C _s	
Rh ₆ _3	C ₁		Rh ₈ _5	C _{2v}	
Rh ₆ _4	C _s		Rh ₈ _6	C _{2v}	
Rh ₇ _1	C _{2v}		Rh ₈ _7	C _s	

(Stable isomers are mentioned in original manuscript)