

Supporting Information

DFT and Machine Learning Guided Investigation into the Design of Dual-Atom Catalysts on New $\alpha - 2$ Graphyne

Chandra Chowdhury*¹, Karthikraja Esackraj^{1,2}

¹Advanced Materials Laboratory,
CSIR-Central Leather Research Institute (CSIR-CLRI),
Sardar Patel Road, Adyar,
Chennai 600 020, India
Email: pc.chandra12@gmail.com

²Academy of Scientific and Innovative Research (AcSIR),
Ghaziabad-201002, India

Venkatesan Subramanian^{2,3}

³Indian Institute of Technology Madras,
Sardar Patel Road, Adyar,
Chennai 600 036, India

August 10, 2024

Table S1: Bond lengths (\AA) of different DACs.

System	Bond Length (\AA)
Sc-Sc	3.1
Sc-Ti	3.02
Sc-V	3.01
Sc-Cr	3.01
Sc-Mn	3.08
Sc-Fe	3.06
Sc-Co	3.15
Sc-Ni	3.31
Sc-Cu	3.06
Sc-Zn	2.78

Table S2: Amount of charge transfer from meta-metal dimer to surface. For example we have chosen here TiM complexes.

Metal (M)	TiM
Ti	2.92
V	2.62
Cr	2.48
Mn	2.31
Fe	1.98
Co	1.95
Ni	1.74
Cu	1.75
Zn	1.85

Table S3: Electronegativity of elements. Comparing the table with Table S2, it is seen that charge transfer from metal to system follows the electronegativity trend.

Element	Electronegativity
Sc	1.36
Ti	1.54
V	1.63
Cr	1.66
Mn	1.55
Fe	1.83
Co	1.88
Ni	1.91
Cu	1.90
Zn	1.65
Y	1.22
Zr	1.33
Nb	1.60
Mo	2.16
Tc	1.90
Ru	2.20
Rh	2.28
Pd	2.20
Ag	1.93
Cd	1.69
Hf	1.30
Ta	1.50
W	2.36
Re	1.90
Os	2.20
Ir	2.20
Pt	2.28
Au	2.54
Hg	2.0

Table S4: Metal bulk and gas phase energy results for the calculation of cohesive energies.

Metal	EM, bulk	EM, gas	ΔE_{coh} -cal
Sc	-6.72	-8.03	-2.10
Ti	-2.47	-4.62	-5.56
V	-9.10	-3.64	-5.46
Cr	-9.90	-5.14	-4.76
Mn	-9.15	-5.15	-4.00
Fe	-8.42	-3.38	-5.04
Co	-7.12	-1.83	-5.29
Ni	-5.48	-1.25	-4.23
Cu	-4.02	-0.24	-3.78
Y	-6.52	-8.45	-1.50
Zr	-2.34	-5.02	-6.11
Nb	-10.51	-3.18	-7.33
Mo	-10.82	-4.58	-6.24
Tc	-10.92	-9.55	-3.40
Ru	-2.47	-7.52	-7.08
Rh	-7.42	-1.37	-6.05
Pd	-5.45	-1.47	-3.98
Ag	-2.72	-0.20	-2.51
Hf	-9.85	-3.34	-6.51
Ta	-12.08	-3.66	-8.42
W	-12.90	-4.53	-8.37
Re	-12.93	-4.61	-8.32
Os	-11.45	-2.92	-8.53
Ir	-9.05	-1.57	-7.48
Pt	-6.40	-0.60	-5.80
Au	-3.25	-0.18	-3.0