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On the H_2 Interaction on Transition Metal Adatoms Supported on Graphene: A Systematic Density Functional Study

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Table S1: Adsorption energies, E_{ads}, in eV/atom, of Transition Metal (*TM*) adatoms supported on graphene, as obtained combining Perdew-Burke-Ernzerhof (*PBE*) exchange-correlation functional with Grimme D2 correction, Grimmed D3, D3 with Becke-Jonson damping (*D3BJ*), and Tkatchenko-Scheffler (*TS*) corrections.

TM	D2	D3	D3BJ	TS
Sc	1.47	1.32	1.63	1.64
Ti	2.17	2.03	2.36	2.21
V	1.88	1.83	2.15	2.00
Cr	0.47	0.33	0.69	0.46
Mn	0.40	0.25	0.58	0.37
Fe	1.04	0.86	1.16	0.99
Co	1.41	1.01	1.29	1.37
Ni	1.98	1.57	1.90	1.91
Cu	0.53	0.41	0.70	0.46
Zn	0.21	0.24	0.49	0.23
Y	1.71	1.49	1.80	1.77
Zr	2.48	2.26	2.59	2.40
Nb	1.68	1.40	1.78	2.27
Mo	0.48	0.26	0.66	0.44
Tc	1.41	1.21	1.60	1.56
Ru	1.91	1.71	2.04	1.87
Rh	2.01	1.90	1.95	1.94
Pd	1.47	1.28	1.61	1.29
Ag	0.35	0.27	0.55	0.26
Cd	0.26	0.26	0.51	0.28
La	2.04	1.35	0.51	—
Hf	1.94	1.65	1.96	1.84
Ta	2.15	1.44	1.76	1.76
W	0.84	0.86	1.18	0.72
Re	0.36	0.36	0.36	0.36
Os	1.33	1.13	1.38	—
Ir	1.52	1.30	1.62	0.98

Pt	1.91	1.79	2.04	1.76
Au	0.54	0.36	0.65	0.38
Hg	0.34	0.28	0.49	0.26

Table S2: Summary of PBE-D3 calculated results of H_2 adsorption on 3*d*, 4*d*, and 5*d* TM adsorbed on graphene, including those adsorption modes not being the lowest in energy, their adsorption energy, E_{ads}, H_2 bond length, *d*(HH), mean H-TM bond length, $\bar{d}$(MH), overall H_2 Bader charge, Q_{H_2}, TM adatom net Bader charge, Q_{TM}, and total magnetic moment of the system, μ. Energies are in kJ mol^{-1}, distances in Å, Q in *e*, and μ in μ_B. For site notation, see main article.

TM	**Site**	E_{ads} **/kJ mol^{-1}**	***d*(HH) /Å**	$\bar{d}$**(MH) /Å**	Q_{H_2} **/e**	Q_{TM} **/e**	μ□/μ□
Sc	K	30.58	0.83	2.05	-0.22	1.27	2.06
Ti	K	55.93	0.81	2.00	-0.19	1.41	3.06
V	P	7.87	0.75	4.41	-0.01	0.99	4.18
Cr	D	33.98	2.42	1.64	-1.02	1.20	4.03
Fe	P	7.57	0.75	5.22	0.00	0.83	2.00
Co	P	27.35	0.75	5.22	0.00	0.65	0.98
Y	P	8.66	0.75	5.65	-0.01	1.08	0.75
Zr	P	6.72	0.75	4.84	-0.02	0.38	3.02
Nb	P	0.70	0.75	4.49	-0.01	0.82	4.04
Mo	D	92.20	2.50	1.73	-1.29	1.54	4.03
Ru	P	8.53	0.75	4.33	-0.01	0.65	2.00
Rh	P	9.50	0.75	4.26	-0.01	0.45	0.99
La	K	26.18	0.85	2.27	-0.24	1.39	0.24
	P	3.80	0.76	3.11	0.00	1.21	0.32
Hf	K	41.95	0.85	2.05	-0.27	1.82	3.06
	P	8.69	0.76	3.13	-0.03	1.65	3.02
Ta	K	88.26	0.91	1.94	-0.44	1.78	3.11
W	P	9.79	0.75	3.51	-0.01	0.5	5.61