

Supporting Information

for

Structure and Dynamics of Co and Ru Adatoms and Nanoclusters on
Tungsten Dichalcogenide Monolayers

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Section S1: Adsorption geometries

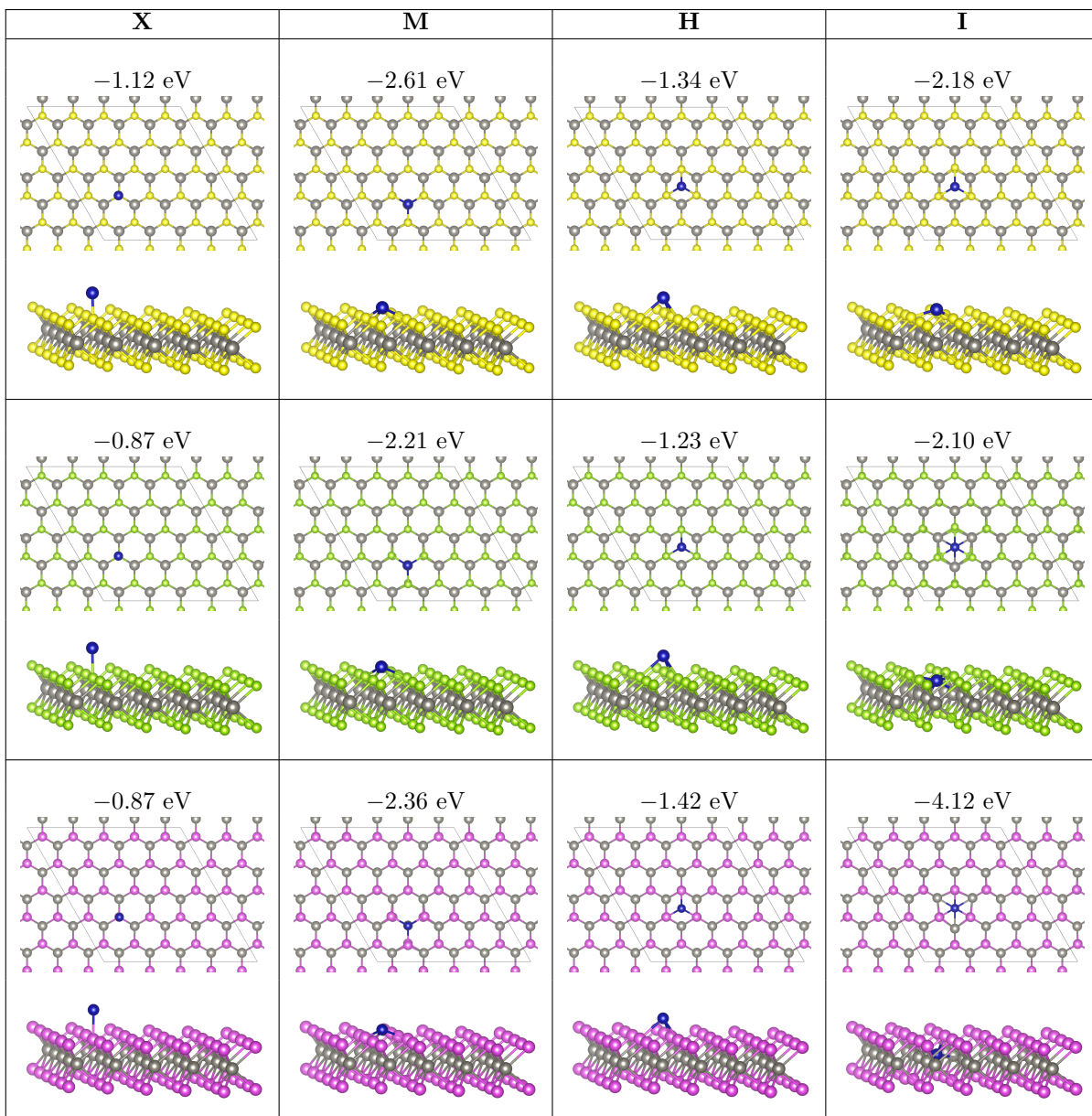


Figure S1: Single atom adsorption modes on WX_2 for Co. **X**, **M**, **H** and **I** refer to the adsorption sites described in the main text

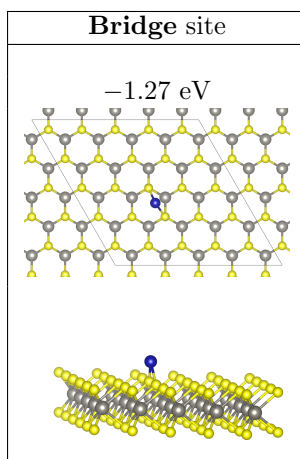


Figure S2: Relaxed adatom adsorption structure on the bridge site for Co on WS₂.

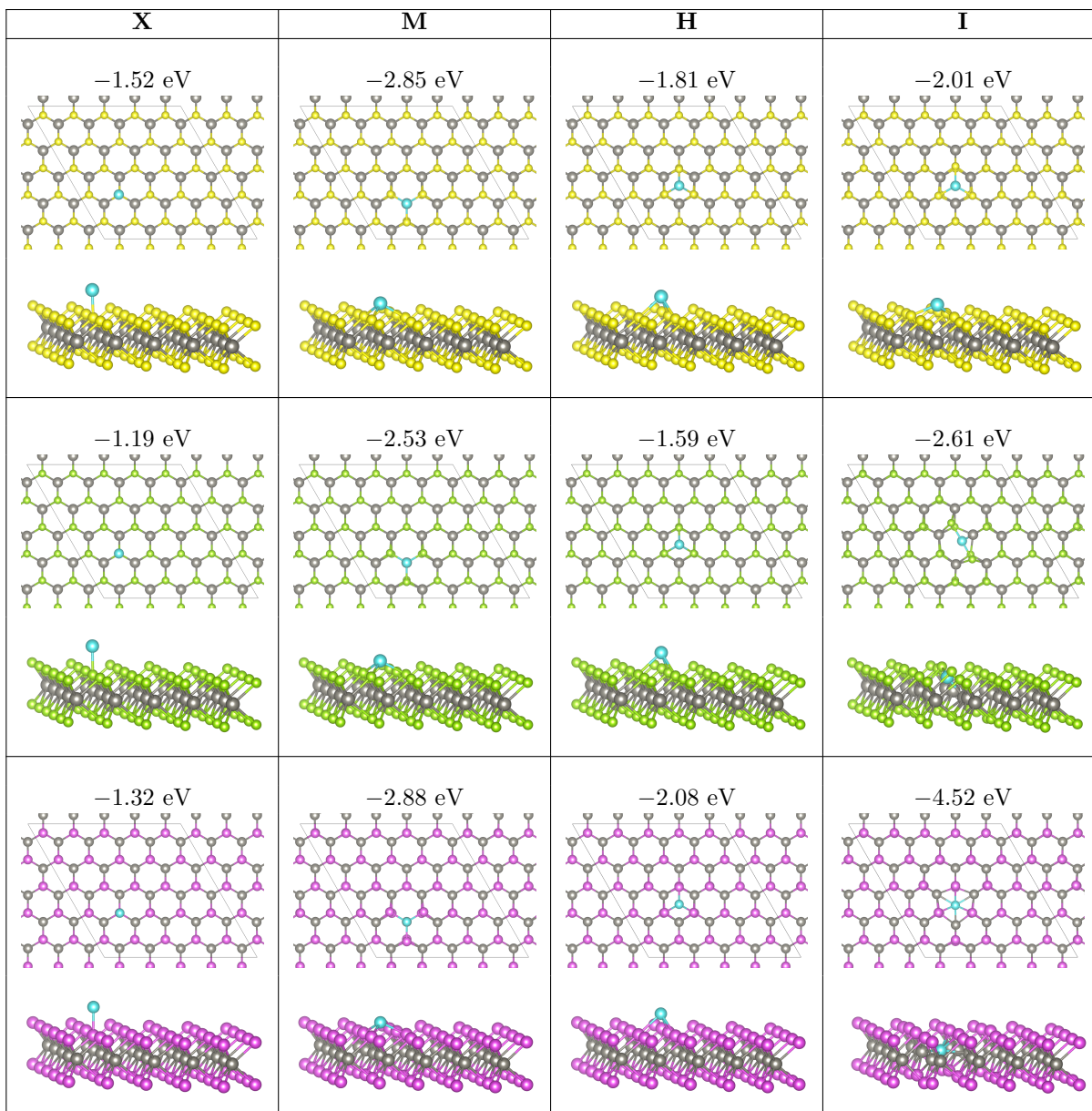


Figure S3: Single atom adsorption modes on WX_2 for Ru. **X**, **M**, **H** and **I** refer to the adsorption sites described in the main text

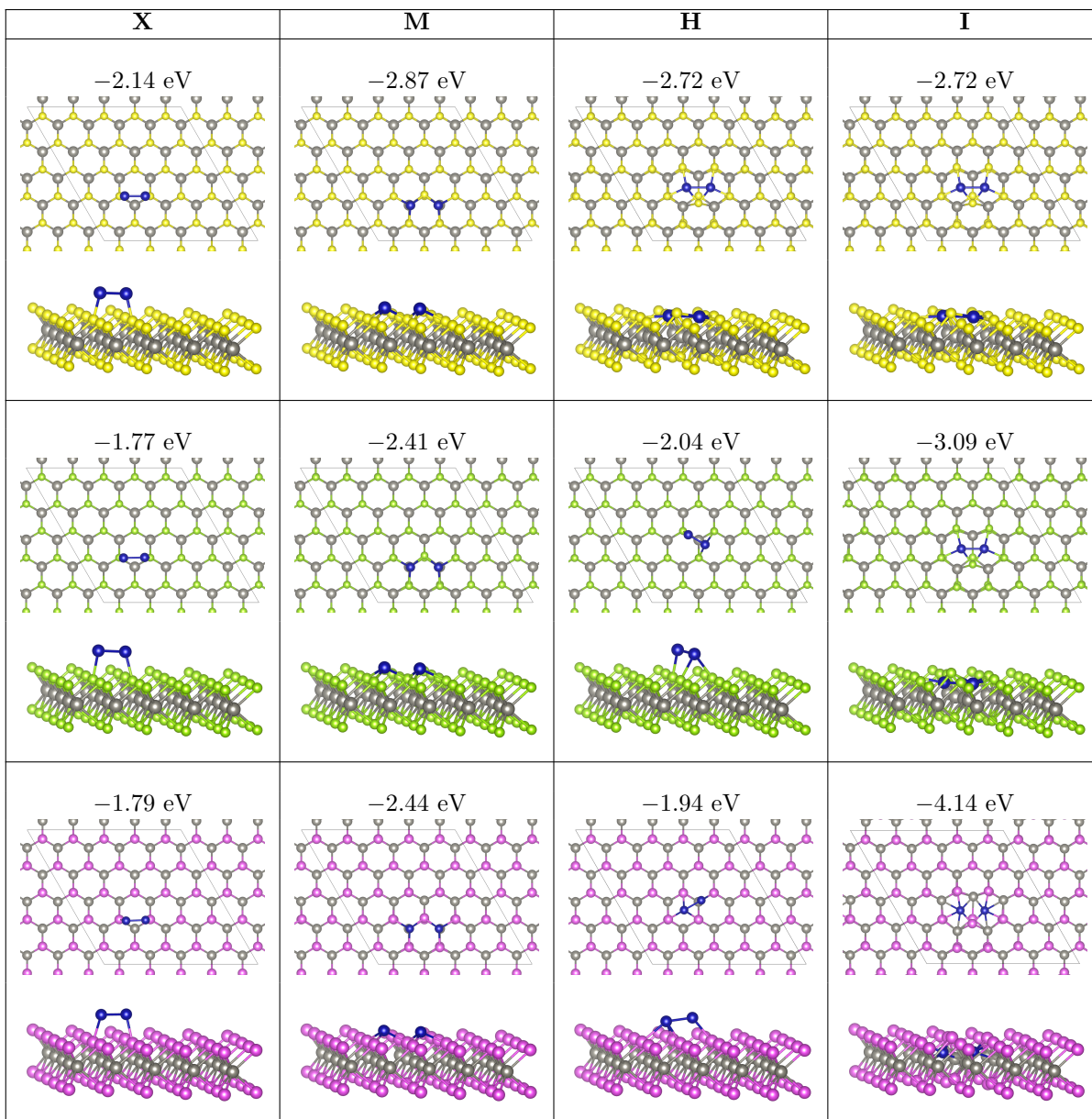


Figure S4: Adsorption structures for 2 Co atoms in the **neighbouring** adsorption modes. Note that all **neighbouring** adsorption at site **H** resulted in atoms migrating to sites other than site **H**.

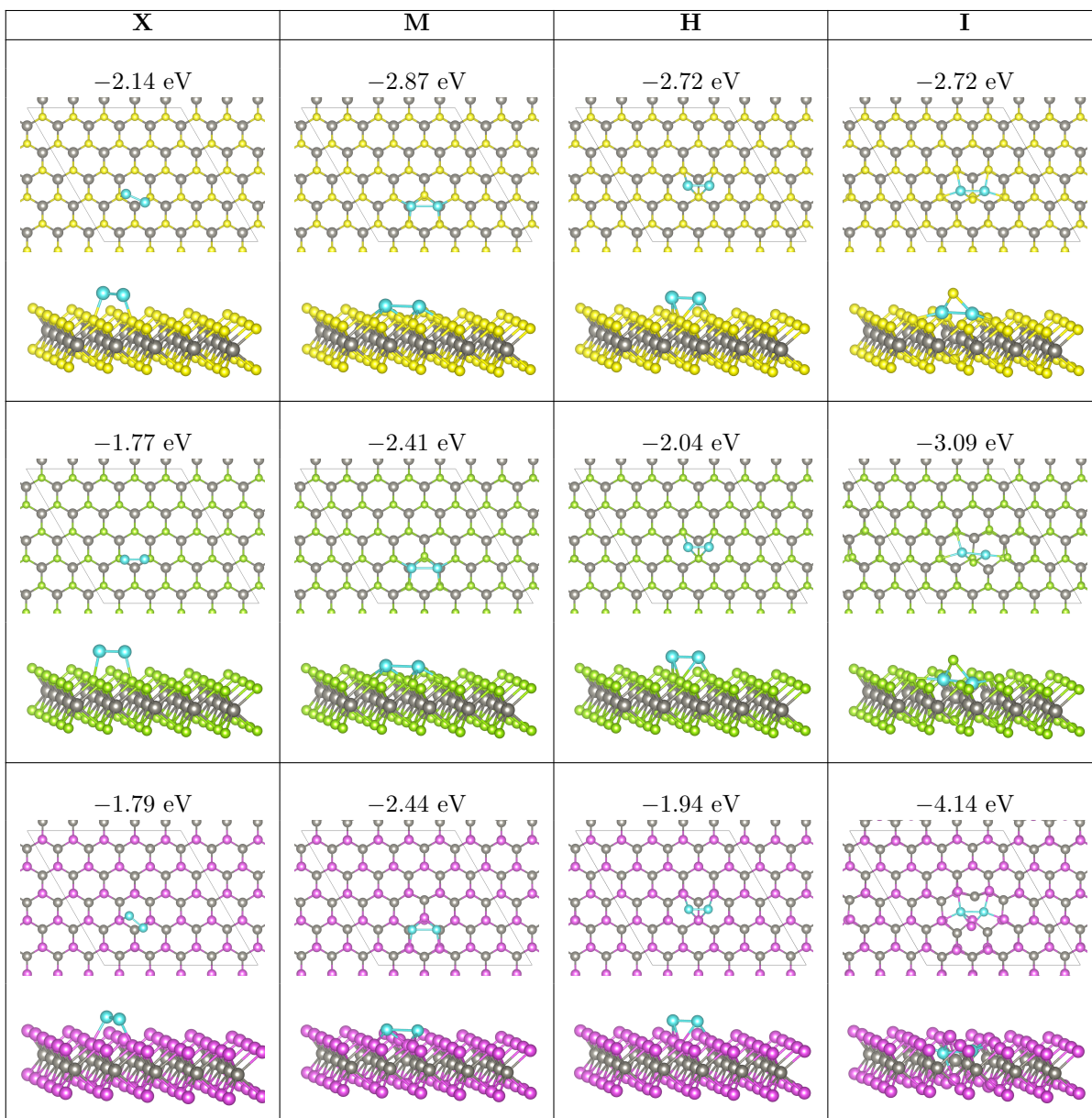


Figure S5: Adsorption structures for 2 Ru atoms in the **neighbouring** adsorption modes.

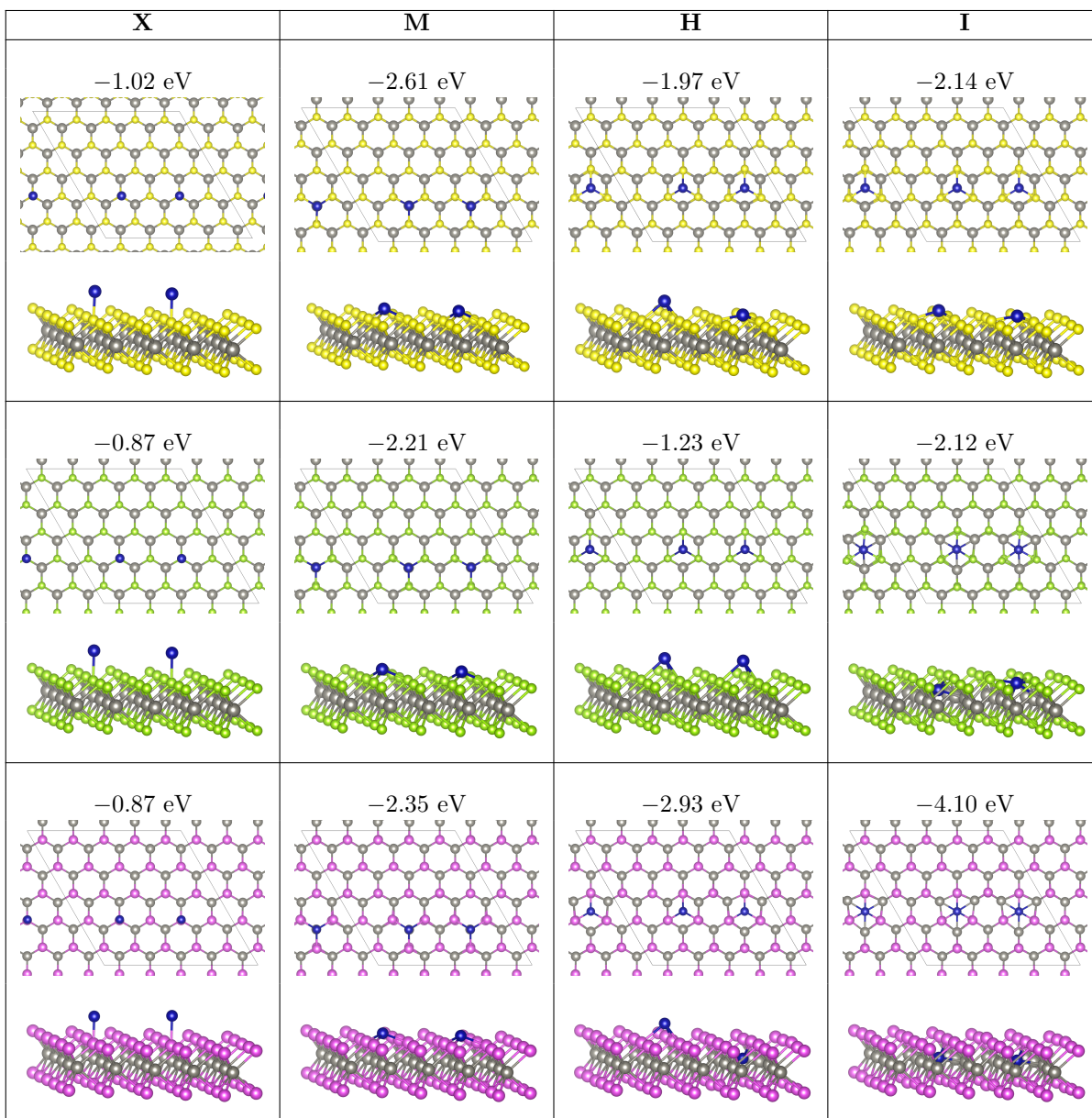


Figure S6: Adsorption structures for 2 Co atoms in the **separated** adsorption modes.

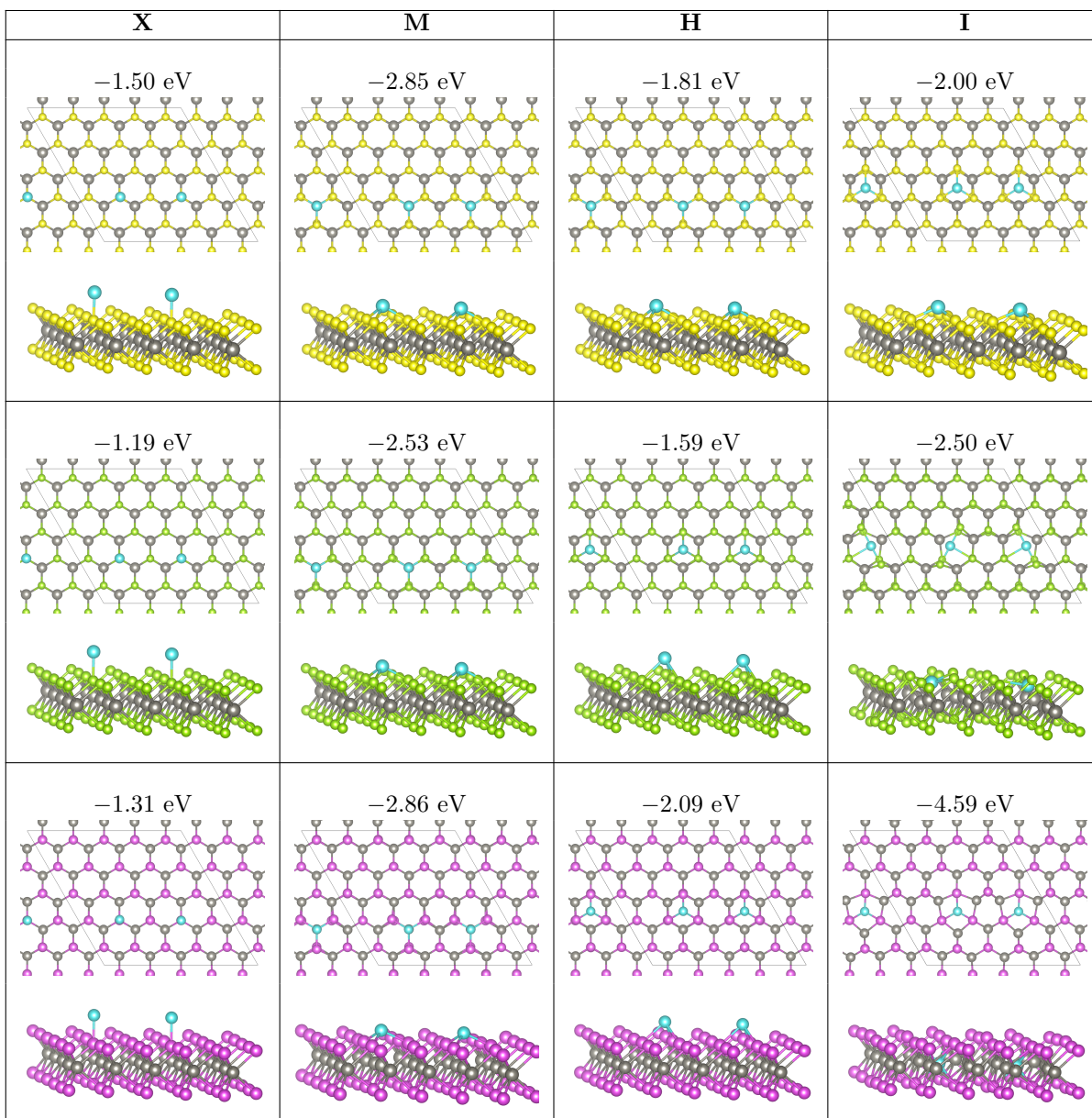


Figure S7: Adsorption structures for 2 Ru atoms in the **separated** adsorption modes.

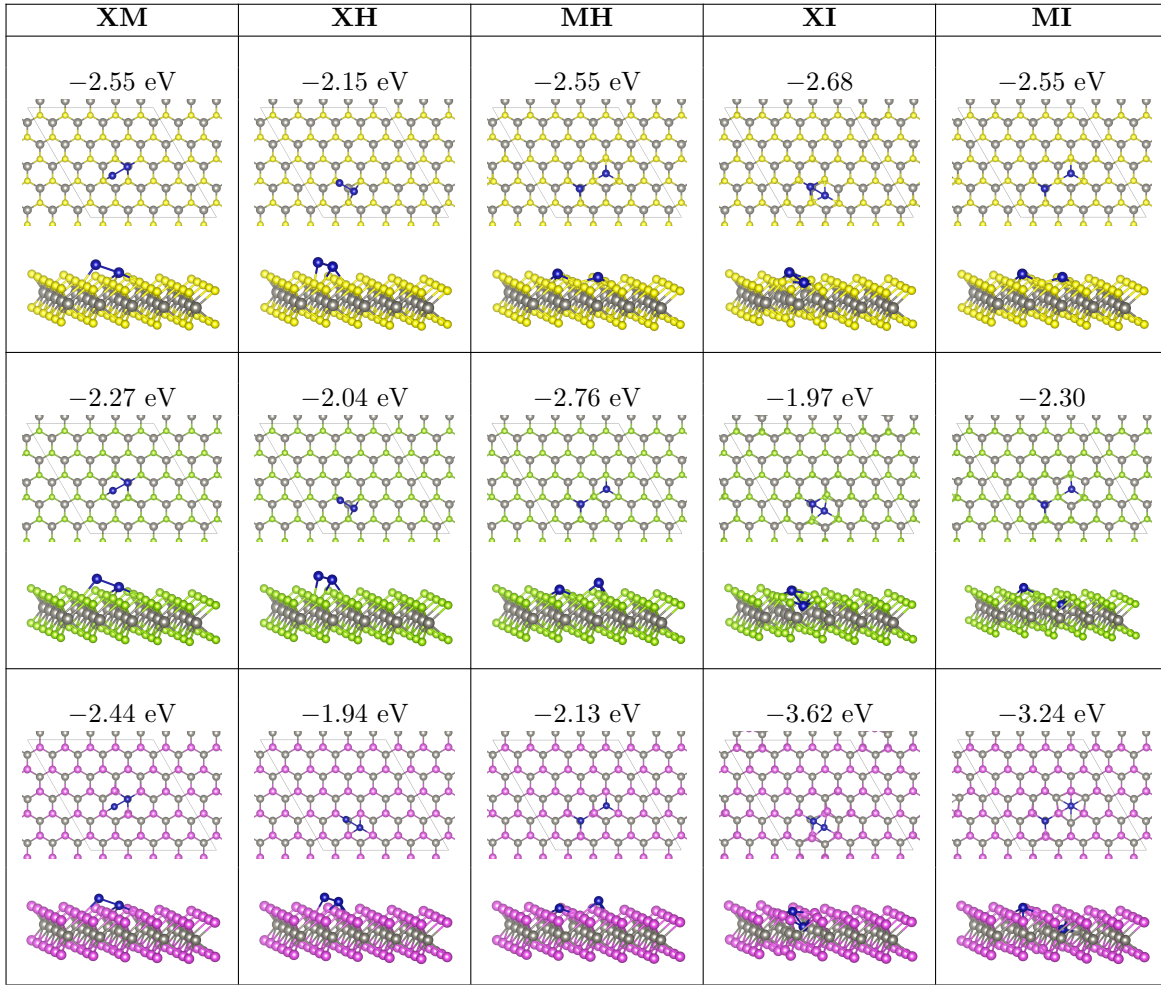


Figure S8: Adsorption structures for 2 Co atoms in the **Non-equivalent** adsorption modes.

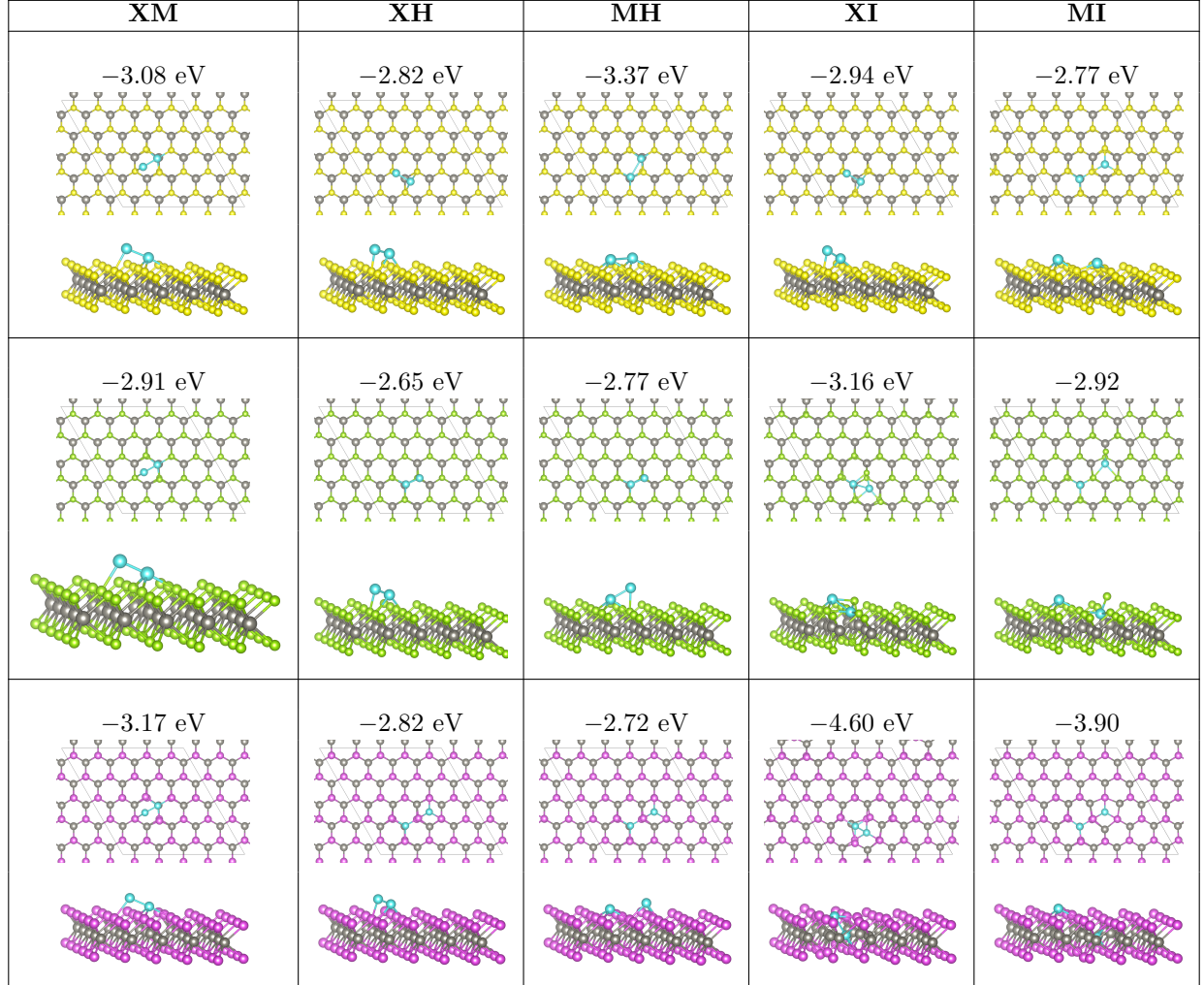


Figure S9: Adsorption structures for 2 Co atoms in the **Non-equivalent** adsorption modes.

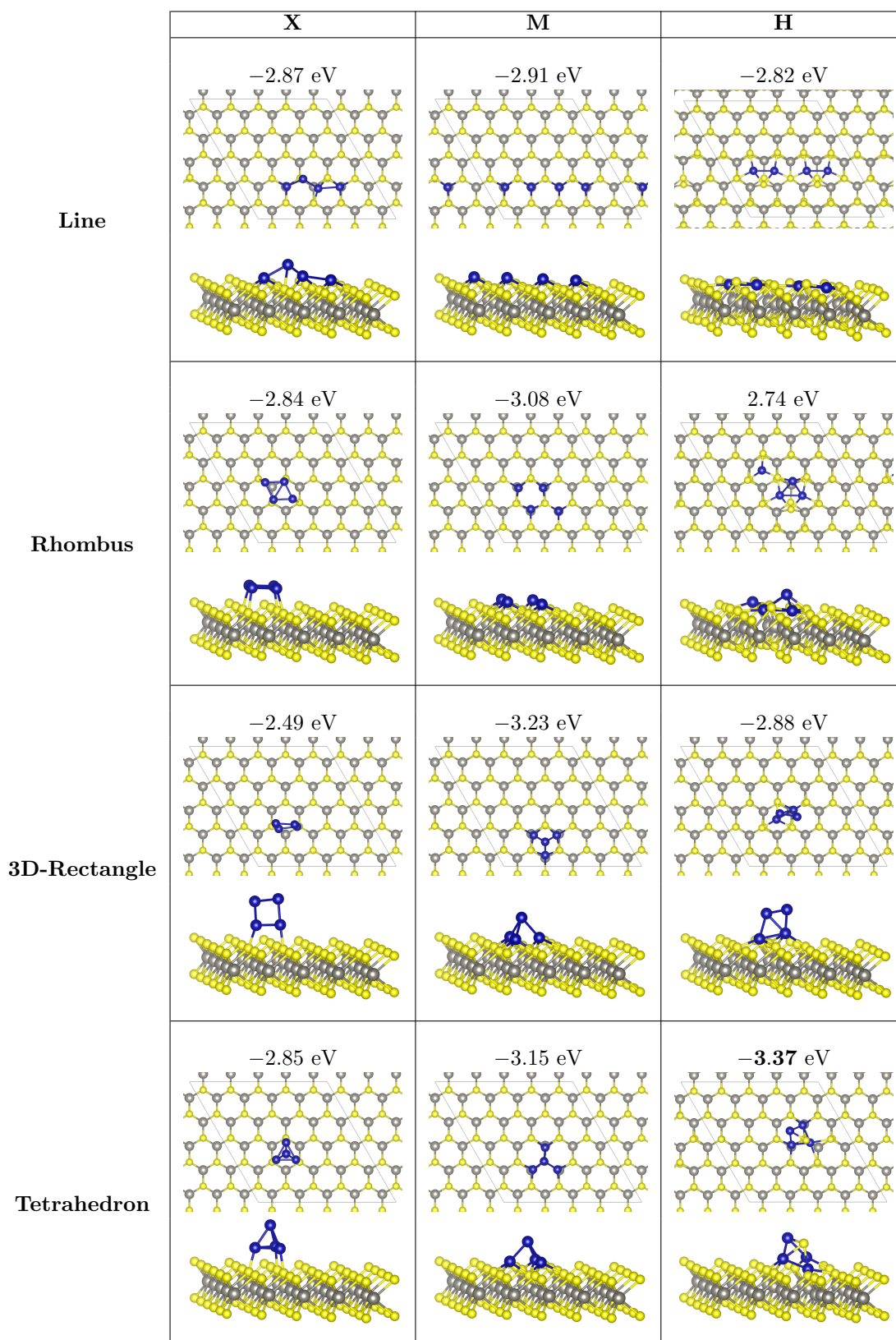


Figure S10: Co four atom adsorption structures on WS₂

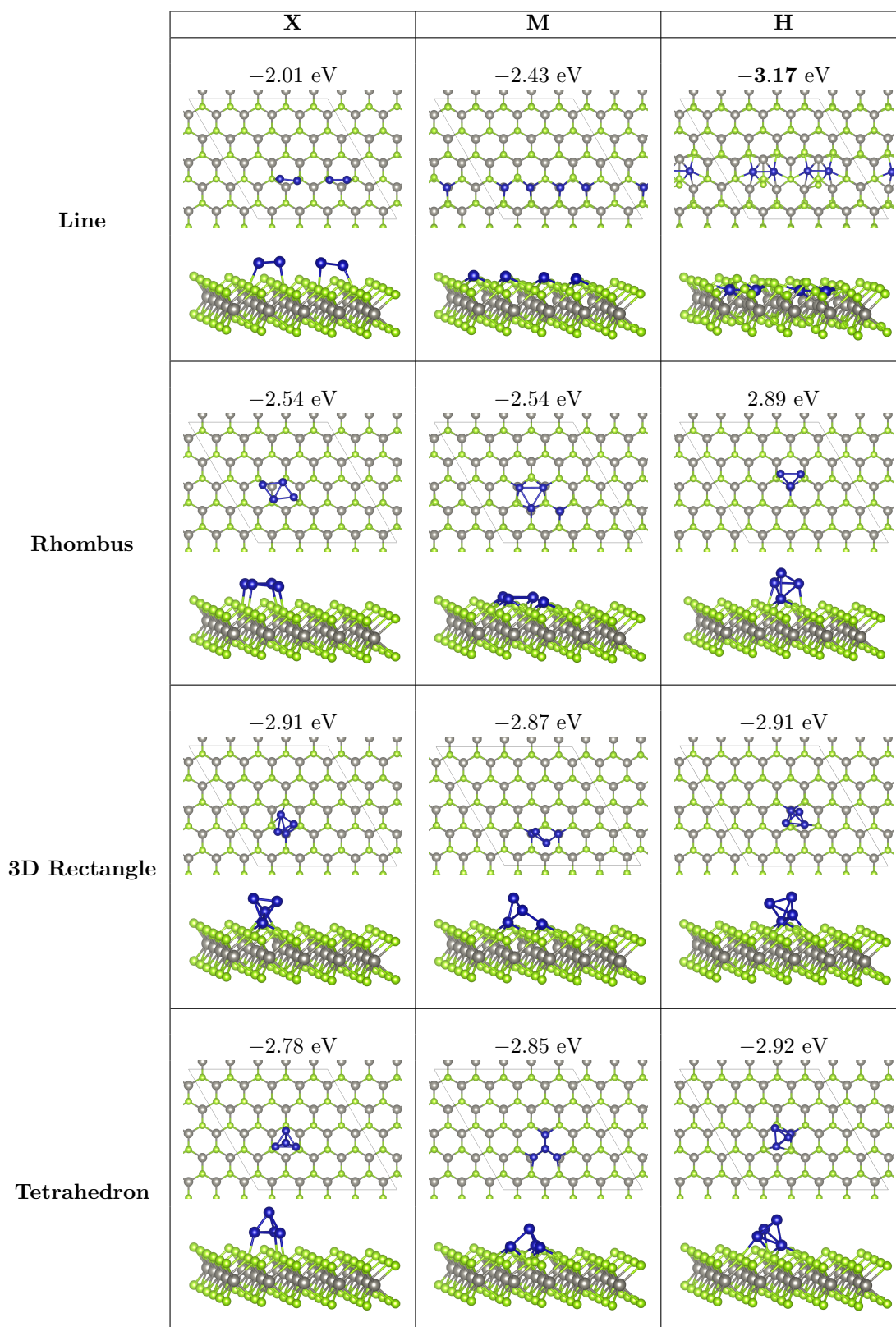


Figure S11: Co four atom adsorption structures on WSe₂

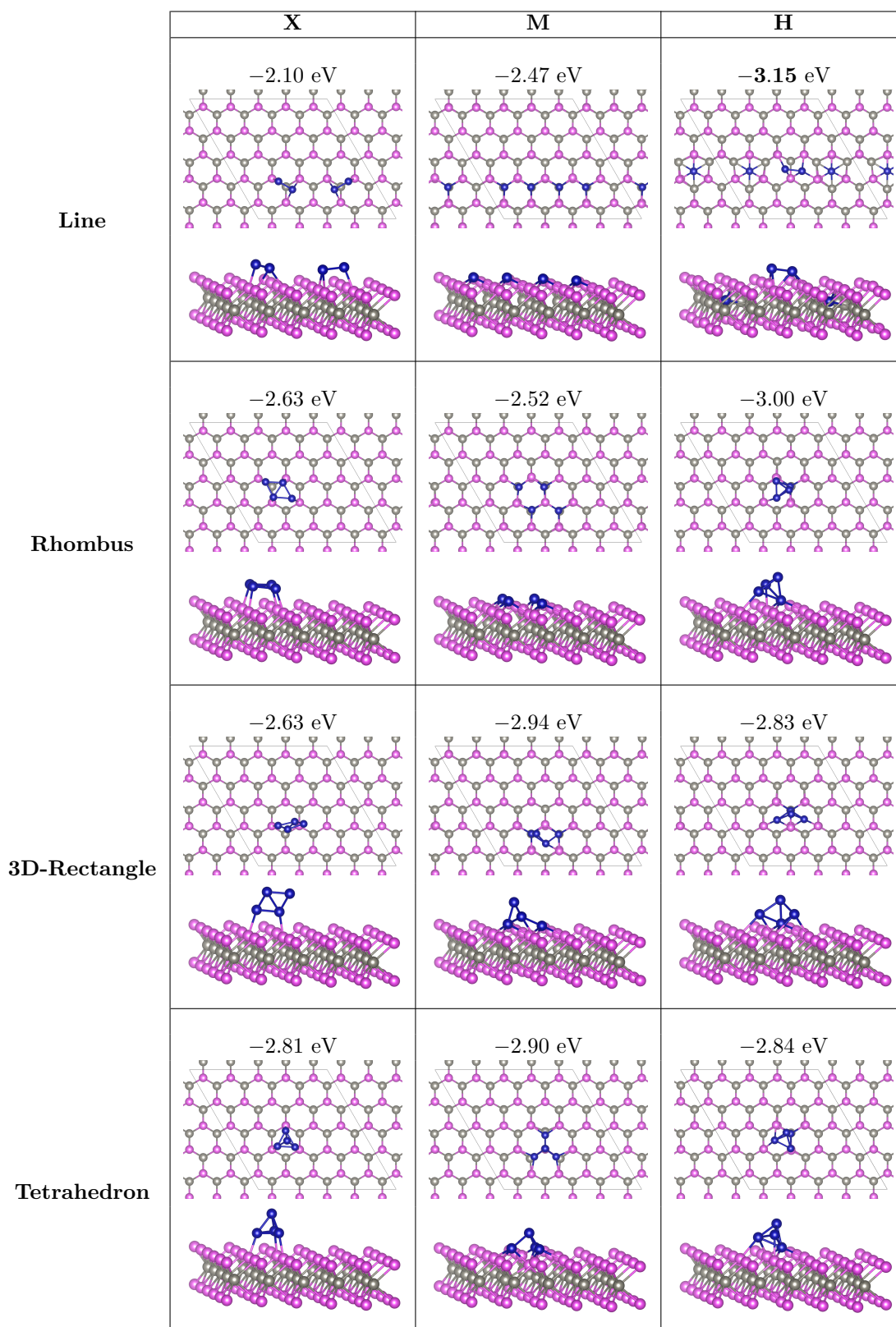


Figure S12: Co four atom adsorption structures on WTe_2

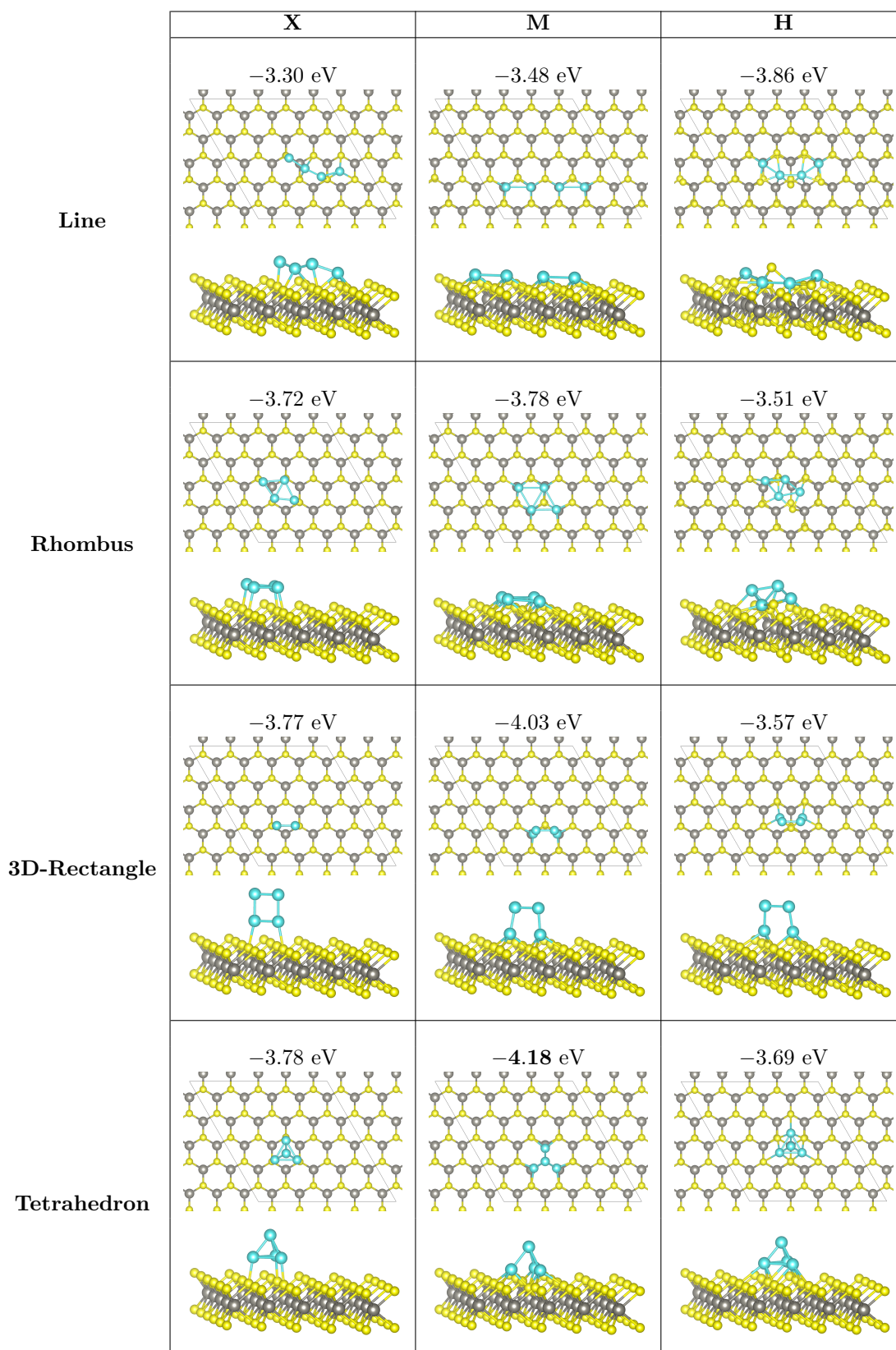


Figure S13: Ru four atom adsorption structures on WS₂
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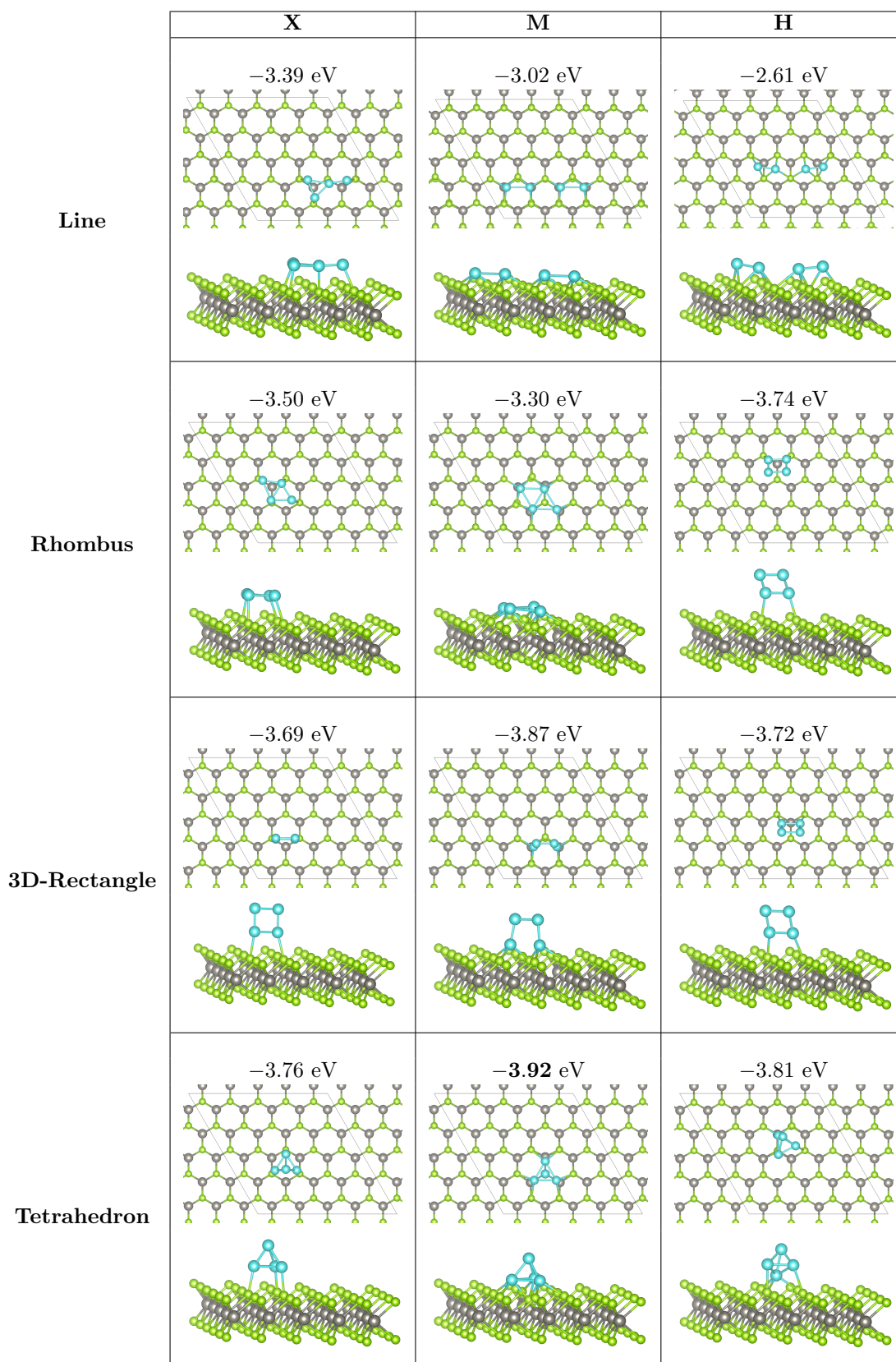


Figure S14: Ru four atom adsorption structures on WSe₂

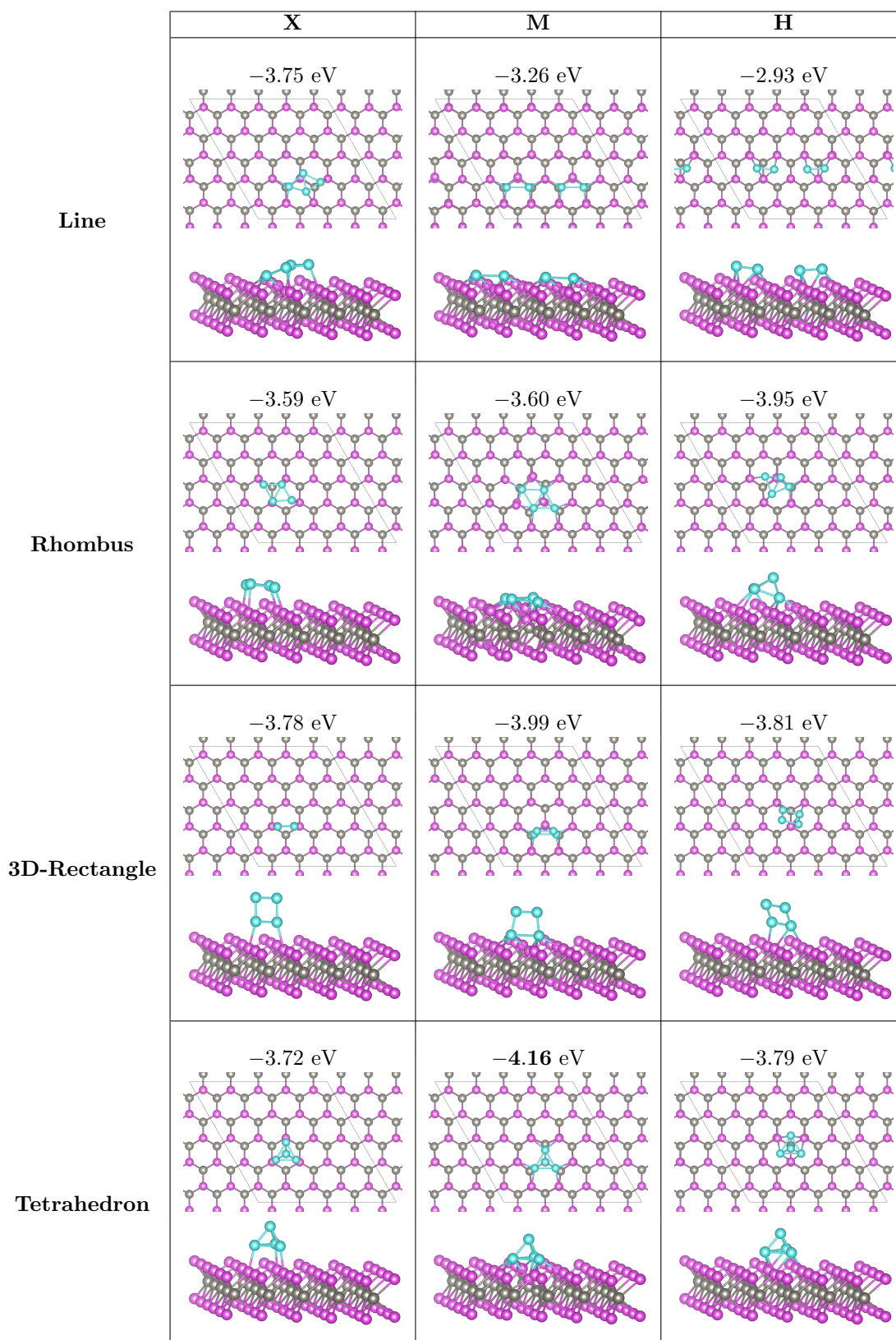


Figure S15: Ru four atom adsorption structures on WTe_2

Section S2: Additional data on geometry and electronic structure

Co	WS ₂				WSe ₂				WTe ₂			
Energy type	X	M	H	I	X	M	H	I	X	M	H	I
Binding	-2.14	-2.87	-2.72	-2.72	-1.77	-2.41	-2.04	-3.09	-1.79	-2.44	-1.94	-4.14
Metal-Metal	-1.46	-0.59	-0.94	-0.94	-1.32	-0.76	-1.50	-1.17	-1.29	-0.28	-1.28	-0.72
Metal-Substrate	-0.68	-2.48	-3.49	-3.49	-0.46	-1.91	-0.55	-3.88	-0.51	-2.32	-0.69	-4.93
Distortion	0.01	0.20	1.71	1.71	0.01	0.27	0.01	1.97	0.01	0.16	0.02	1.51
Ru	WS ₂				WSe ₂				WTe ₂			
Energy type	X	M	H	I	X	M	H	I	X	M	H	I
Binding	-2.85	-3.37	-2.75	-3.76	-2.70	-2.94	-2.58	-4.25	-2.88	-3.20	-2.92	-5.18
Metal-Metal	-1.73	-1.34	-2.03	-1.79	-1.79	-1.30	-1.67	-1.64	-1.81	-1.17	-1.59	-1.40
Metal-Substrate	-1.14	-2.25	-0.77	-5.33	-0.91	-1.94	-0.95	-6.63	-1.14	-2.38	-1.39	-6.07
Distortion	0.02	0.22	0.05	3.36	0.01	0.31	0.05	4.02	0.08	0.36	0.06	2.29

Table S1: Disaggregated adsorption energy for **Neighbouring 2** atom adsorption for both metals on all three monolayers on all three monolayers

Co	WS ₂				WSe ₂				WTe ₂			
Energy type	X	M	H	I	X	M	H	I	X	M	H	I
Binding	-1.02	-2.61	-1.97	-2.14	-0.87	-2.21	-1.23	-2.12	-0.87	-2.35	-2.93	-4.10
Metal-Metal	-0.22	-0.22	-0.22	-0.22	0.07	-0.22	-0.19	-0.21	0.15	0.16	0.17	0.14
Metal-Substrate	-0.80	-2.60	-2.07	-2.48	-0.94	-2.32	-1.07	-3.59	-1.05	-2.89	-3.61	-5.37
Distortion	0.00	0.21	0.31	0.56	0.00	0.32	0.04	1.68	0.03	0.38	0.51	1.12
Ru	WS ₂				WSe ₂				WTe ₂			
Energy type	X	M	H	I	X	M	H	I	X	M	H	I
Binding	-1.50	-2.85	-1.81	-2.00	-1.19	-2.53	-1.59	-2.15	-1.31	-2.86	-2.09	-4.59
Metal-Metal	0.61	0.50	0.61	0.50	0.53	0.72	0.50	0.61	0.62	1.09	0.71	-0.10
Metal-Substrate	-2.12	-3.65	-2.59	-3.15	-1.74	-3.73	-2.22	-7.58	-1.98	-4.50	-2.92	-6.50
Distortion	0.01	0.30	0.17	0.66	0.02	0.48	0.13	4.48	0.05	0.55	0.12	2.01

Table S2: Disaggregated adsorption energy for **Separated** 2 atom adsorption for both metals on all three monolayers on all three monolayers

Co	X	M	H	I
WS ₂	2.00	2.12	2.38	2.06
WSe ₂	2.37	2.24	2.52	2.23
WTe ₂	2.55	2.39	2.67	2.54
Ru	X	M	H	I
WS ₂	2.13	2.26	2.37	2.21
WSe ₂	2.29	2.37	2.51	2.36
WTe ₂	2.46	2.51	2.64	2.66

Table S3: Average metal-X distance for single atom adsorption of Co and Ru on all three monolayer Å

Co	WS ₂					WSe ₂					WTe ₂				
Energy type	XM	XH	MH	XI	MI	XM	XH	MH	XI	MI	XM	XH	MH	XI	MI
Binding	-2.55	-2.15	-2.55	-2.68	-2.55	-2.27	-2.04	-1.97	-2.76	-2.30	-2.44	-1.94	-2.13	-3.62	-3.24
Metal-Metal	-1.28	-1.45	-0.41	-1.30	-0.41	-1.30	-1.49	-0.42	-1.37	-0.28	-1.31	-1.29	-0.33	-1.26	-0.23
Metal-Substrate	-1.38	-0.72	-2.44	-2.58	-2.43	-1.13	-0.56	-1.72	-2.93	-3.00	-1.29	-0.67	-1.98	-3.67	-3.76
Distortion	0.10	0.02	0.29	1.20	0.29	0.15	0.01	0.16	1.53	0.98	0.16	0.02	0.18	1.31	0.75
Ru	WS ₂					WSe ₂					WTe ₂				
Energy type	XM	XH	MH	XI	MI	XM	XH	MH	XI	MI	XM	XH	MH	XI	MI
Binding	-3.08	-2.82	-3.37	-2.94	-2.77	-2.91	-2.65	-2.77	-3.16	-2.92	-3.17	-2.82	-2.72	-4.60	-3.90
Metal-Metal	-1.81	-1.64	-1.30	-2.05	-0.31	-1.96	-1.34	-1.86	-1.66	1.06	-1.95	-1.69	0.08	-1.35	0.80
Metal-Substrate	-1.43	-1.21	-2.29	-1.12	-2.93	-1.18	-1.35	-1.07	-3.96	-6.80	-1.47	-1.17	-3.06	-5.37	-5.99
Distortion	0.16	0.03	0.22	0.22	0.47	0.23	0.04	0.16	2.46	2.82	0.25	0.04	0.27	2.12	1.29

Table S4: Disaggregated adsorption energy for **non-equivalent** 2 atom adsorption for both metals on all three monolayers on all three monolayers

Energy type	Adsorption Configuration	WS ₂			WSe ₂			WTe ₂		
		X	M	H	X	M	H	X	M	H
Binding	Line	-2.87	-2.91	-2.82	-2.01	-2.43	-3.17	-2.10	-2.47	-3.15
Metal-Metal		-1.75	-1.00	-1.33	-1.52	-0.94	-1.29	-1.49	-0.66	-0.82
Metal-Substrate		-1.21	-2.05	-3.25	-0.50	-1.76	-3.91	-0.63	-1.96	-2.93
Distortion		0.09	0.14	1.76	0.01	0.27	2.03	0.02	0.16	0.60
Binding	Rhombus	-2.84	-3.08	-2.74	-2.54	-2.54	-2.89	-2.63	-2.52	-3.00
Metal-Metal		-2.32	-1.25	-1.50	-2.25	-1.29	-2.11	-2.23	-0.71	-2.06
Metal-Substrate		-0.54	-1.98	-2.44	-0.29	-1.45	-0.83	-0.40	-1.96	-1.01
Distortion		0.01	0.15	1.19	0.01	0.19	0.06	0.01	0.15	0.07
Binding	3D-rectangle	-2.49	-3.23	-2.88	-2.91	-2.87	-2.91	-2.63	-2.94	-2.83
Metal-Metal		-2.26	-1.93	-2.24	-2.18	-2.08	-2.11	-2.29	-2.05	-2.19
Metal-Substrate		-0.23	-1.39	-0.86	-0.79	-0.86	-0.86	-0.36	-1.00	-0.73
Distortion		0.00	0.09	0.22	0.06	0.08	0.06	0.01	0.10	0.09
Binding	Tetrahedron	-2.85	-3.15	-3.37	-2.78	-2.85	-2.92	-2.81	-2.90	-2.84
Metal-Metal		-2.07	-1.80	-2.13	-2.23	-1.86	-2.11	-2.10	-1.86	-2.20
Metal-Substrate		-0.79	-1.44	-2.79	-0.56	-1.14	-0.87	-0.71	-1.28	-0.72
Distortion		0.01	0.09	1.55	0.01	0.15	0.06	0.01	0.24	0.08

Table S5: Disaggregated adsorption energy for four atom Co adsorption on all three monolayers

Energy type	Adsorption Configuration	WS ₂			WSe ₂			WTe ₂		
		X	M	H	X	M	H	X	M	H
Binding	Line	-3.30	-3.48	-3.86	-3.39	-3.02	-2.61	-3.75	-3.26	-2.93
Metal-Metal		-2.62	-1.39	-2.11	-2.93	-1.36	-1.97	-2.90	-1.23	-2.01
Metal-Substrate		-0.71	-2.27	-4.33	-0.50	-1.95	-0.68	-0.95	-2.40	-0.98
Distortion		0.03	0.19	2.58	0.04	0.29	0.05	0.09	0.36	0.06
Binding	Rhombus	-3.72	-3.78	-3.51	-3.50	-3.30	-3.74	-3.59	-3.60	-3.95
Metal-Metal		-2.99	-2.06	-2.91	-2.99	-2.31	-3.37	-2.92	-2.26	-3.01
Metal-Substrate		-0.75	-1.88	-1.75	-0.53	-1.34	-0.38	-0.68	-1.96	-1.02
Distortion		0.03	0.16	1.14	0.02	0.34	0.01	0.01	0.62	0.09
Binding	3D-rectangle	-3.77	-4.03	-3.57	-3.69	-3.87	-3.72	-3.78	-3.99	-3.81
Metal-Metal		-3.37	-3.06	-3.19	-3.37	-3.09	-3.38	-3.35	-3.03	-3.36
Metal-Substrate		-0.41	-1.06	-0.49	-0.32	-0.90	-0.35	-0.44	-1.13	-0.46
Distortion		0.01	0.09	0.11	0.00	0.12	0.01	0.01	0.16	0.02
Binding	Tetrahedron	-3.78	-4.18	-3.69	-3.76	-3.92	-3.81	-3.72	-4.16	-3.79
Metal-Metal		-3.01	-2.91	-3.01	-3.22	-2.94	-3.09	-2.98	-2.91	-2.97
Metal-Substrate		-0.78	-1.39	-0.72	-0.54	-1.17	-0.78	-0.74	-1.55	-0.87
Distortion		0.01	0.12	0.04	0.01	0.19	0.06	0.01	0.30	0.04

Table S6: Disaggregated adsorption energy for four atom Ru adsorption on all three monolayers

Table S7: Total (M_{tot}) and atom-projected (m_i) magnetic moments in μ_B for Co adsorption structures on each monolayer.

n	Config.	WS ₂		WSe ₂		WTe ₂	
		M_{tot}	$\{m_i\}$	M_{tot}	$\{m_i\}$	M_{tot}	$\{m_i\}$
1	X	1.00	–	3.00	–	3.00	–
	M	1.00	–	1.00	–	1.00	–
	H	3.01	–	3.00	–	3.01	–
	I	1.00	–	1.00	–	0.89	–
2	X	4.00	1.84, 1.85	–0.08	–1.82, 1.72	0.07	1.83, –1.70
	M, neighbouring	2.00	0.96, 0.96	2.00	1.01, 1.01	2.00	1.00, 0.97
	H	2.00	0.76, 0.72	4.00	1.87, 2.02	0.00	–1.48, 1.92
	I	–	–	1.94	0.78, 0.77	2.01	0.85, 0.64
	X, separated	6.01	2.19, 2.19	6.00	2.20, 2.20	2.00	–1.50, 2.21
	M, separated	2.00	0.94, 0.94	2.00	1.00, 0.97	2.00	0.97, 0.98
	H, separated	2.00	0.94, 0.78	5.92	1.99, 1.99	2.07	1.72, 0.03
	I, separated	–	–	1.55	–0.17, 1.17	–0.09	0.38, –0.36
	X-M	2.00	1.82, 0.08	2.00	0.06, 1.84	2.00	0.32, 1.73
	X-H	4.00	1.76, 1.96	4.00	1.87, 2.01	0.00	1.49, –1.92
	M-H	2.00	0.84, 1.01	2.04	1.67, 0.13	1.91	1.64, –0.05
	X-I	–	–	–2.00	–1.23, –0.70	1.90	0.77, 1.03
	M-I	–	–	2.05	0.16, 1.54	–2.02	–0.43, –1.11
4	X, Line	4.00	0.21, 1.69, 1.48, 0.60	8.00	1.86, 1.99, 1.98, 1.90	0.00	–1.89, –1.99, 1.99, 1.88
	M, Line	4.00	0.87, 0.99, 1.00, 0.92	4.00	0.99, 0.99, 1.01, 1.01	4.00	1.05, 1.05, 0.93, 0.92
	H, Line	4.00	0.67, 0.67, 0.77, 0.78	1.88	0.02, 0.76, 0.81, –0.04	–4.09	–1.55, –1.60, –0.07, –0.46
	X, Rhombus	8.06	1.79, 1.94, 1.78, 1.94	0.05	–1.78, 1.73, 1.74, –1.68	–4.04	–1.70, 1.57, –1.74, –1.93
	M, Rhombus	4.00	0.32, 1.09, 1.04, 1.08	4.00	0.32, 1.15, 1.08, 1.16	4.00	1.10, 0.74, 1.12, 0.91
	H, Rhombus	4.00	0.77, 0.71, 0.68, 1.18	6.00	1.97, 0.48, 1.74, 1.74	5.95	1.62, 0.64, 1.93, 1.78
	X, Rhombus, 3D	3.99	1.69, 1.43, 1.92, –1.32	5.99	0.47, 1.64, 1.96, 1.86	8.00	1.84, 1.74, 2.01, 2.07
	M, Rhombus, 3D	4.02	0.78, 0.78, 1.95, 0.79	–6.00	–0.81, –0.97, –2.06, –1.90	–6.00	–0.95, –0.92, –1.83, –2.06
	H, Rhombus, 3D	6.00	0.72, 0.95, 2.05, 2.09	–6.00	–0.46, –1.63, –1.81, –2.00	–2.00	–0.09, –1.83, –1.90, 1.78
	X, Tetrahedron	4.02	1.69, 1.68, 1.69, –1.51	5.91	1.61, 1.61, 1.54, 1.65	5.95	1.55, 1.62, 1.62, 1.64
	M, Tetrahedron	–2.00	0.66, –0.32, –0.32, –2.04	4.00	0.91, 0.96, 0.28, 1.96	–4.00	–0.99, –0.99, –0.24, –1.94
	H, Tetrahedron	0.02	0.39, 1.20, 0.38, –1.91	5.99	1.64, 0.65, 1.77, 1.92	–1.99	–1.61, 1.34, 0.03, –1.79
	H, Tetrahedron, Xvac	6.00	1.56, 1.46, 1.56, 0.88	0.05	0.01, 0.01, 0.00, 0.01	0.00	0.00, 0.00, 0.00, 0.00

Table S8: Total (M_{tot}) and atom-projected (m_i) magnetic moments in μ_B for Ru adsorption structures on each monolayer.

n	Config.	WS ₂		WSe ₂		WTe ₂	
		M_{tot}	$\{m_i\}$	M_{tot}	$\{m_i\}$	M_{tot}	$\{m_i\}$
0	vacancy (post-relax.)	-0.06	—	0.00	—	0.00	—
1	X	2.00	—	1.99	—	1.97	—
	M	2.00	—	2.00	—	2.02	—
	H	2.00	—	2.00	—	2.00	—
	I	2.00	—	0.00	—	0.00	—
2	X	2.03	0.93, 0.93	4.04	1.53, 1.52	2.02	0.86, 0.94
	M, neighbouring	1.98	0.62, 0.62	2.06	0.67, 0.68	2.08	0.65, 0.66
	H	1.90	0.86, 0.86	2.05	0.92, 0.94	2.07	0.93, 0.92
	I	2.01	0.57, 0.55	0.00	0.00, 0.00	0.00	0.00, 0.00
	X, separated	4.00	1.75, 1.75	3.99	1.77, 1.77	3.99	1.78, 1.79
	M, separated	4.00	1.17, 1.17	4.00	1.21, 1.21	4.02	1.17, 1.17
	H, separated	4.00	1.42, 1.42	4.00	1.52, 1.54	4.00	1.45, 1.46
	I, separated	4.00	1.38, 1.38	0.00	0.00, 0.00	1.05	0.17, 0.18
	X-M	4.01	2.43, 0.62	3.99	0.65, 2.37	4.02	0.70, 2.31
	X-H	4.05	1.30, 1.65	1.95	1.13, 0.54	1.93	0.50, 1.14
	M-H	1.98	0.62, 0.61	2.00	1.43, 0.28	3.96	1.56, 0.98
	X-I	2.07	1.20, 0.54	0.04	0.06, -0.01	0.00	0.00, 0.00
	M-I	1.97	0.58, 0.63	2.05	0.05, 1.11	2.06	0.66, 0.04
4	X, Line	0.00	-0.14, -0.11, 0.20, 0.17	3.95	1.01, 0.75, 0.72, 0.98	4.02	0.03, 1.41, 0.97, 1.04
	M, Line	3.99	0.70, 0.55, 0.55, 0.70	4.03	0.66, 0.66, 0.68, 0.68	4.01	0.65, 0.66, 0.69, 0.69
	H, Line	1.98	0.23, 0.23, 0.49, 0.50	4.06	0.74, 0.75, 0.98, 0.98	4.07	0.84, 0.84, 0.94, 0.94
	X, Rhombus	1.94	0.36, 0.62, 0.51, 0.24	5.99	1.67, 2.04, 0.14, 1.05	8.02	2.12, 1.66, 1.49, 1.46
	M, Rhombus	2.01	0.18, 0.57, 0.09, 0.57	4.05	0.50, 1.02, 0.20, 1.02	0.01	0.51, -0.00, -0.49, -0.00
	H, Rhombus	0.00	0.00, 0.00, 0.00, 0.00	1.96	0.73, 1.04, -0.29, 0.17	1.96	-0.82, 0.12, 1.73, 0.47
	X, Rhombus, 3D	4.07	0.85, 0.85, 0.95, 0.96	4.01	0.56, 0.57, 1.11, 1.11	4.08	0.84, 0.84, 0.96, 0.97
	M, Rhombus, 3D	1.99	-0.06, -0.06, 0.98, 0.98	1.98	-0.06, -0.07, 0.98, 0.98	2.00	-0.05, -0.05, 0.98, 0.98
	H, Rhombus, 3D	1.94	-0.07, -0.06, 0.98, 0.98	4.02	0.62, 0.62, 1.10, 1.10	1.94	-0.65, -0.00, 1.23, 0.94
	X, Tetrahedron	6.04	1.24, 1.28, 1.25, 1.69	3.95	0.71, 0.71, 0.61, 1.38	6.06	1.28, 1.28, 1.29, 1.53
	M, Tetrahedron	1.95	0.09, 0.09, 0.08, 1.26	2.00	0.10, 0.10, 0.10, 1.20	1.98	0.09, 0.09, 0.09, 1.06
	H, Tetrahedron	0.04	0.34, 0.37, 0.30, -0.74	4.06	1.03, 1.17, -0.06, 1.36	1.98	0.34, 0.34, 0.72, 0.20

Table S9: Energy difference ΔE_{spin} (eV) between the spin-relaxed and fixed high-spin states for Co adsorption structures. Negative values indicate the relaxed spin state is more stable. Blank entries were not computed.

n	Config.	WS ₂	WSe ₂	WTe ₂
1	X	−0.10	0.00	0.00
	M	−0.81	−0.61	−0.66
	H	−0.97	−0.01	0.00
	I	–	−0.88	−0.62
2	X	−0.40	–	–
	X-H	−0.31	–	–
	X-M	−0.69	–	–
	X, separated	0.00	–	–
	M-H	−0.98	–	–
	M, neighbouring	−0.96	–	–
	M, separated	−0.81	–	–
	H	−0.08	–	–
	H, separated	−0.95	–	–
4	X, Line	−0.71	−0.21	−0.24
	X, Rhombus	−0.45	–	–
	X, Rhombus, 3D	−0.10	–	–
	X, Tetrahedron	−0.43	–	–
	M, Line	−0.95	−0.71	−0.60
	M, Rhombus	−0.99	–	–
	M, Rhombus, 3D	−0.81	–	–
	M, Tetrahedron	−0.72	–	–
	H, Line	−0.74	−0.82	−0.38
	H, Rhombus	−0.74	–	–
	H, Tetrahedron	−0.38	–	–

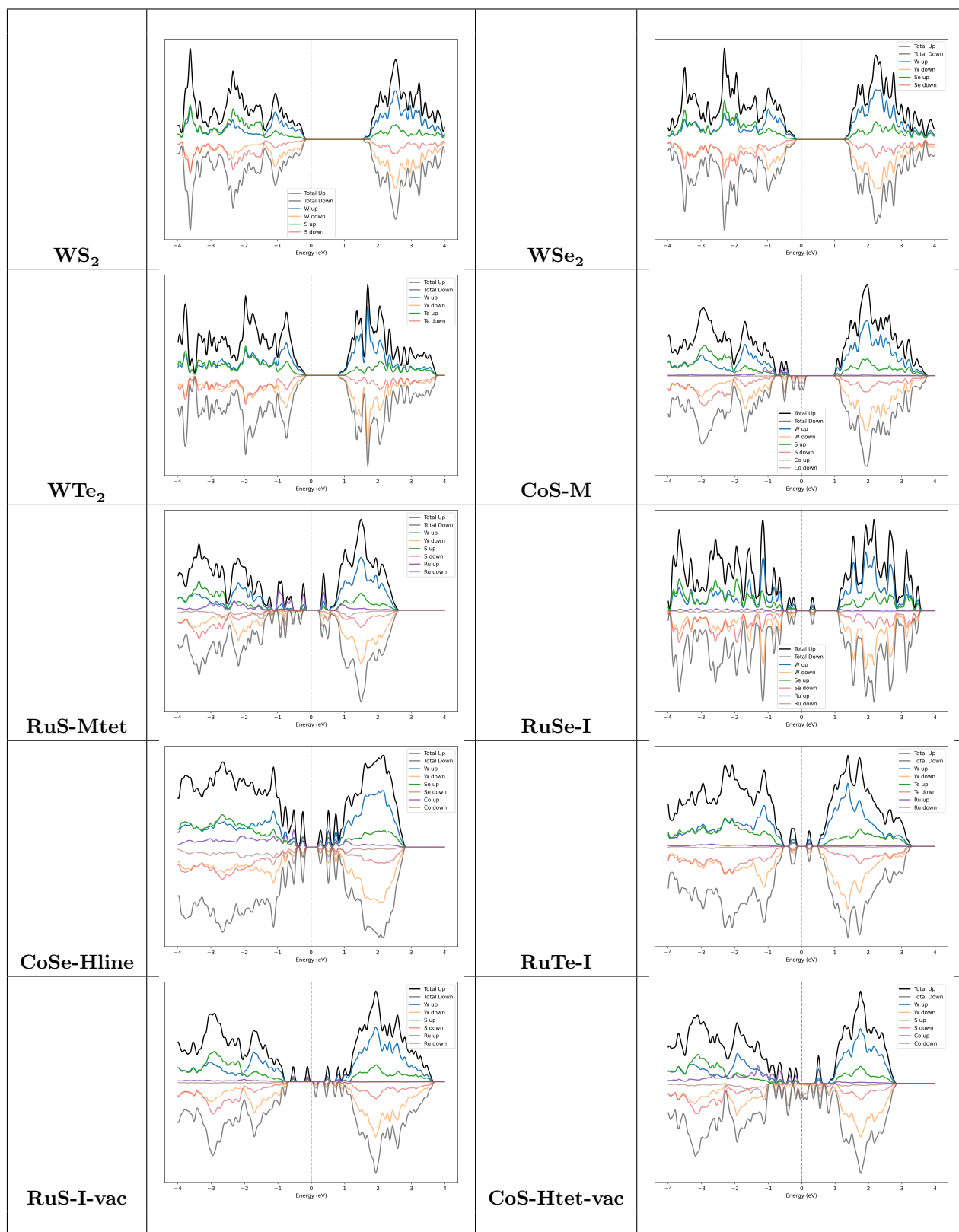


Figure S16: Computed electronic density of states of selected Co and Ru adsorption structures on WX_2

Section S3: Plane-wave energy cut-off convergence for the aiMD calculations

Section S3.1: 250 eV cut-off justification

Ab initio molecular dynamics (aiMD) simulations were performed with a reduced plane-wave cut-off of 250 eV to access longer time-scales with the available computing resources, whereas all 0 K relaxations and NEB calculations used a cut-off of 450 eV. This allows us to use aiMD to explore the configurational space of metal-nanocluster morphology. All total energies which are obtained from the 0 K or NEB calculations use a 450 eV as the energies are well converged at this cut-off. To confirm that the 250 eV cut-off is adequate for configurational exploration, we assess the convergence of the energies, forces (magnitude and direction) between 250 and 450 eV below.

For each system, five uncorrelated frames from representative aiMD trajectories were selected. A single-point calculation was performed on each frame at a range of cut-off energies, and the differences in energy, force magnitude, and force direction relative to the same frame at 450 eV were computed. This was then averaged over the five frames. The most stable one- and four-atom structures for which aiMD was performed were used; in Figures S17 and S18 the labels CoX/RuX denote Co/Ru adsorbed on the corresponding WX₂ monolayer. The panels of Figure S17 are grouped by metal-monolayer combination, and the panels of Figure S18 by chalcogen species.

At a 250 eV cut-off the total energy is offset by between 5 and 17 meV/atom relative to 450 eV, depending on the metal-monolayer combination. The standard deviation of this offset across frames (Figure S18d) shows that this is a constant shift arising from the change in basis-set size with cut-off, rather than a fluctuating error. Because all energy differences are reported at 450 eV, this constant offset does not affect the results as the gradient of the potential energy surface determines behaviour at temperature, rather than the absolute value. Figure S18d further shows that the magnitude of the offset is governed largely by the chalcogen species present.

The errors in both force magnitude and force direction are small at 250 eV for all systems (Figure S18b). A larger force error is seen at 400 eV for Co@WS₂ and Co@WTe₂, but it remains below the 0.05 eV/Å threshold used for the NEB calculations. This error arises from a single outlier frame in each case and the maximum error across all frames is 0.03 eV/Å. The energies converge monotonically, with no spike at 400 eV, and the force directions do not deviate from those at 450 eV.

These tests show that a 250 eV cut-off is suitable for the configurational exploration of metal nanoclusters, allowing the potential energy landscape to be sampled efficiently while adsorption energies and activation barriers for the selected structures are reported from relaxations and NEB calculations at 450 eV.

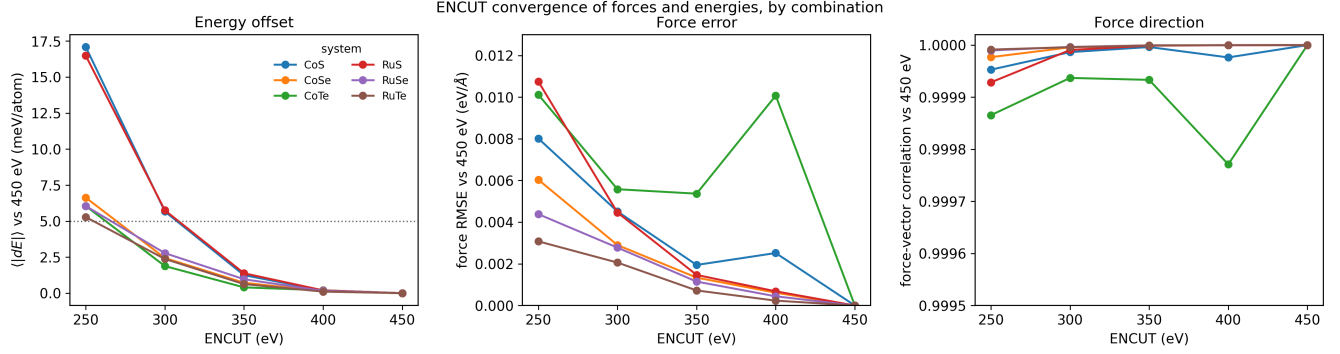


Figure S17: Plane-wave cut-off (ENCUT) convergence of energies and forces relative to 450 eV, grouped by metal-monolayer combination (CoX/RuX denotes Co/Ru on the WX_2 monolayer). (a) Mean absolute energy offset per atom. (b) Force RMSE. (c) Force-vector correlation with the 450 eV reference. All quantities are averaged over five uncorrelated aiMD frames per system.

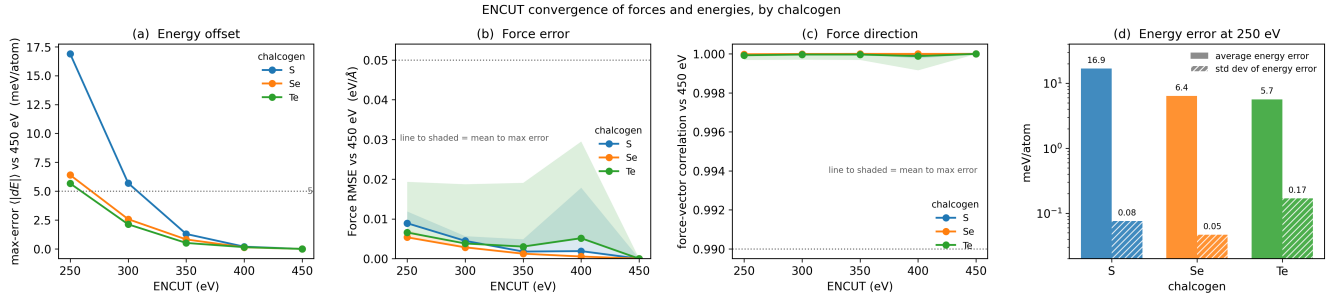


Figure S18: Plane-wave cut-off (ENCUT) convergence of energies and forces relative to 450 eV, grouped by chalcogen species. (a) Maximum absolute energy offset per atom. (b) Force RMSE, shaded region spans the mean to the maximum error. (c) Force-vector correlation with the 450 eV reference. (d) Average energy error and its standard deviation at 250 eV, by chalcogen. All line-plot quantities are averaged over five uncorrelated aiMD frames per system.