Supplementary Information: Two-dimensional Metal Dichalcogenides and Oxides for Hydrogen Evolution: A Computational Screening Approach

Mohnish Pandey,[†] Aleksandra Vojvodic,[‡] Kristian S. Thygesen,[†,¶] and Karsten W. Jacobsen[*,†]

Center for Atomic-scale Materials Design, Department of Physics, Technical University of Denmark, DK - 2800 Kongens Lyngby, Denmark, SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory 2575 Sand Hill Road, California 94025, United States, and Center for Nanostructured Graphene (CNG), Department of Physics, Technical University of Denmark, DK - 2800 Kongens Lyngby, Denmark

E-mail: kwj@fysik.dtu.dk

[*]To whom correspondence should be addressed

[†]Center for Atomic-scale Materials Design, Department of Physics, Technical University of Denmark, DK - 2800 Kongens Lyngby, Denmark

[‡]SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory 2575 Sand Hill Road, California 94025, United States

[¶]Center for Nanostructured Graphene (CNG), Department of Physics, Technical University of Denmark, DK - 2800 Kongens Lyngby, Denmark

Table 1: Adsorption energies ΔH^H_{ads} (in eV) and lattice constants a (in angstrom) of the compounds with 2H structure and 2×2 unitcell as shown in Figure 4.

2H-MX_2	ΔH^H_{ads}	a	2H-MX_2	ΔH^H_{ads}	a	2H-MX_2	ΔH^H_{ads}	a
ScS_2	-0.072	7.56	$ScSe_2$	0.205	7.88	CoS_2	-0.114	6.45
$CoSe_2$	0.425	6.72	RuO_2	-0.986	5.83	RuS_2	-0.231	6.71
$RuSe_2$	0.389	6.94	$RuTe_2$	0.406	7.4	RhS_2	-0.425	6.83
$RhSe_2$	0.075	7.12	$RhTe_2$	0.727	7.57	PdS_2	-0.255	7.81
$PdSe_2$	0.22	8.04	ReO_2	-0.295	5.6	ReS_2	0.897	6.31
$ReSe_2$	1.279	6.9	$ReTe_2$	1.653	7.42	OsS_2	-0.35	6.77
$OsSe_2$	0.409	7.03	$OsTe_2$	1.058	7.5	IrS_2	-0.384	6.85
$IrSe_2$	0.04	7.11	$PtTe_2$	0.573	7.84	PbO_2	-1.778	6.47
$ScTe_2$	0.934	7.26	TiS_2	-0.05	6.72	$TiSe_2$	0.436	6.98
$TiTe_2$	0.683	7.49	VO_2	-1.173	5.53	VS_2	0.216	6.35
VSe_2	0.806	6.71	VTe_2	1.043	7.2	CrO_2	0.259	5.19
CrS_2	1.228	6.09	$CrSe_2$	1.564	6.41	$CrTe_2$	1.447	6.95
$MnSe_2$	1.926	6.72	$MnTe_2$	3.009	7.35	FeO_2	-1.436	5.44
FeS_2	0.347	6.32	$FeTe_2$	1.684	7.15	CoO_2	-1.788	5.52
$CoTe_2$	0.77	7.25	$NiSe_2$	-0.348	7.03	$NiTe_2$	0.693	7.44
ZrS_2	0.108	7.14	$ZrSe_2$	0.511	7.4	$ZrTe_2$	0.698	7.84
NbS_2	-0.038	6.73	$NbSe_2$	0.361	6.94	$NbTe_2$	0.51	7.37
MoO_2	1.263	5.65	MoS_2	1.681	6.35	$MoSe_2$	1.824	6.66
$MoTe_2$	1.742	7.09	$PdTe_2$	0.421	8.05	HfS_2	0.302	7.08
$HfSe_2$	0.643	7.35	$HfTe_2$	0.755	7.82	TaO_2	-0.467	5.96
TaS_2	0.113	6.72	$TaSe_2$	0.498	6.94	$TaTe_2$	0.487	7.39
$IrTe_2$	0.022	7.6	WO_2	1.842	5.68	WS_2	1.95	6.36
WSe_2	2.033	6.66	WTe_2	1.874	7.1	ScO_2	-0.829	6.48

Table 2: Adsorption energies ΔH^H_{ads} (in eV) and lattice constants a (in angstrom) of the compounds with 1T structure and 2×2 unitcell as shown in Figure 4.

1T-MX_2	ΔH^H_{ads}	a	1T-MX_2	ΔH^H_{ads}	a	1T-MX_2	ΔH^H_{ads}	a
CoS_2	-0.008	6.41	$CoSe_2$	0.486	6.71	$CoTe_2$	0.647	7.26
CrO_2	-1.462	5.85	FeO_2	-1.196	5.65	FeS_2	0.354	6.39
$FeSe_2$	0.54	6.76	$FeTe_2$	0.601	7.28	GeO_2	1.561	5.82
GeS_2	0.487	6.87	$GeSe_2$	0.26	7.26	HfO_2	2.104	6.46
HfS_2	1.179	7.3	$HfSe_2$	1.41	7.53	$HfTe_2$	1.318	7.97
IrO_2	-0.59	6.33	IrS_2	-0.137	7.12	$IrSe_2$	0.714	7.43
$IrTe_2$	0.662	7.78	MnO_2	-0.173	5.81	$MnSe_2$	1.042	6.97
$MnTe_2$	2.882	7.48	MoO_2	-0.424	5.83	MoS_2	0.096	6.34
$MoSe_2$	0.643	6.58	$MoTe_2$	0.909	6.98	NbS_2	0.376	6.79
$NbSe_2$	0.714	6.96	$NbTe_2$	0.47	7.29	NiO_2	-0.686	5.71
NiS_2	0.447	6.74	$NiSe_2$	0.756	7.09	$NiTe_2$	0.994	7.56
OsO_2	0.115	6.23	OsS_2	0.999	6.97	$OsTe_2$	1.223	7.72
PbO_2	-1.017	6.84	$PbSe_2$	-0.127	8.02	PdO_2	-0.515	6.23
PdS_2	0.37	7.1	$PdSe_2$	0.813	7.46	$PdTe_2$	0.659	8.05
PtO_2	0.242	6.35	PtS_2	0.839	7.14	$PtSe_2$	1.009	7.49
$PtTe_2$	0.966	8.03	ReO_2	0.997	5.63	ReS_2	1.485	6.16
$ReSe_2$	1.593	6.33	$ReTe_2$	1.531	6.81	RhO_2	-1.285	6.23
RhS_2	-0.151	7.01	$RhSe_2$	0.406	7.18	$RhTe_2$	0.607	7.59
RuO_2	-0.563	6.17	RuS_2	0.509	6.78	$RuSe_2$	0.862	6.92
$RuTe_2$	0.731	7.54	ScO_2	-2.259	6.49	ScS_2	-0.926	7.48
$ScSe_2$	-0.338	7.71	$ScTe_2$	0.57	7.64	SnO_2	0.437	6.51
SnS_2	0.877	7.39	$SnSe_2$	0.778	7.72	$SnTe_2$	0.44	8.24
TaO_2	0.893	6.14	TaS_2	1.041	6.8	$TaSe_2$	0.794	6.99
$TaTe_2$	0.327	7.36	TiO_2	0.218	6.02	TiS_2	0.402	6.89
$TiSe_2$	0.901	7.08	$TiTe_2$	1.083	7.51	VO_2	-0.857	5.82
VS_2	0.522	6.35	VSe_2	0.69	6.74	VTe_2	0.52	7.21
WO_2	-0.58	5.83	WS_2	0.233	6.39	WSe_2	0.789	6.62
WTe_2	0.79	7.0	ZrO_2	1.706	6.49	ZrS_2	0.941	7.35
$ZrSe_2$	1.19	7.58	$ZrTe_2$	1.187	7.96	CoO_2	-1.55	5.68
PbS_2	-0.111	7.68	$CrTe_2$	0.639	7.36	MnS_2	0.469	6.75
CrS_2	-0.089	6.67	$CrSe_2$	0.41	6.87	$OsSe_2$	1.149	7.19