Electronic Supplementary Information for Synergistic Screening of High-Performance TMDs/2D-LHPs Heterostructures for Solar Cells via Deep Learning and DFT

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Table S1 Summary of Power Conversion Efficiency (PCE%) for All TMDs/2D-LHPs Heterostructures. The table presents the bandgap of the heterojunction (E_g eV), donor bandgap (E_g^d eV), open-circuit voltage (V_{OC} eV), and conduction band offset (CBO eV).

Heterostructure	E_g (eV)	E_g^d (eV)	V_{OC} (eV)	CBO (eV)	PCE (%)
$[I(CH_2)_4NH_3]_2PbI_4/MoSSe$	0.99	1.59	1.12	0.17	18.19
$[CH_3(CH_2)_3NH_3]_2SnI_4/WS_2$	1.01	1.95	1.45	0.19	14.12
$[BrC_6H_4(CH_2)_2NH_3]_2PbI_4/WTe_2$	1.01	1.13	0.71	0.12	19.99
$[C_5H_4N(CH_2)NH_3]PbI_4/MoSeTe$	1.02	1.03	0.55	0.18	16.65
$[I(CH_2)_5NH_3]_2PbI_4/WSTe$	1.03	1.94	1.27	0.38	12.36
$[CH_3(CH_2)_3NH_3]_2CsPb_2Br_7/WTe_2$	1.06	2.23	1.90	0.04	11.36
$[CH_3(CH_2)_3NH_3]_2PbBr_4/WTe_2$	1.06	1.84	1.47	0.07	16.87
$(C_{15}H_{31}NH_3)_2PbI_4/MoS_2$	1.07	1.82	1.30	0.21	15.58
$[C_6H_5CH_2NH_3]_2PbBr_4/WTe_2$	1.40	1.48	0.07	0.02	21.95
$[F_2C_6H_9NH_3]_2PbI_4/MoSSe$	1.10	2.02	1.20	0.52	10.31
$(C_{11}H_{23}NH_3)_2PbI_4/MoS_2$	1.12	1.84	1.40	0.14	16.03
$[C_7H_{10}N]_2PbI_4/WSSe$	1.12	1.71	1.28	0.12	17.91
$(C_{13}H_{27}NH_3)_2PbI_4/MoS_2$	1.13	1.84	1.52	0.02	17.50
$[I(CH_2)_6NH_3]_2PbI_4/WSTe$	1.14	2.16	1.58	0.28	10.80
$[C_{12}H_{14}N]_2PbBr_4/MoSSe$	1.15	1.68	1.34	0.04	19.34
$[I(CH_2)_4NH_3]_2PbI_4/MoSe_2$	1.17	1.53	1.01	0.21	18.05
$[CH_3(CH_2)_3NH_3]_2SnI_4/MoSSe$	1.17	1.64	1.32	0.02	20.16
$[C_6H_5CH_2NH_3]_2PbI_4/WSTe$	1.17	1.76	1.24	0.22	16.05
$[C_5H_4N(CH_2)NH_3]PbCl_4/WSTe$	1.18	1.75	1.42	0.03	18.80
$[C_7H_9FN]_2PbCl_4/WSTe$	1.19	2.55	1.97	0.28	6.26
$[CH_3(CH_2)_3NH_3]_2PbI_4/MoS_2$	1.21	1.83	1.33	0.20	15.63
$[CH_3(CH_2)_3NH_3]_2PbI_4/MoS_2$	1.22	1.82	1.29	0.23	15.35

$[I(CH_2)_5NH_3]_2PbI_4/MoSeTe$	1.22	1.99	1.65	0.05	14.81
$[CH_3(CH_2)_5NH_3]_2PbI_4/WSe_2$	1.23	1.76	1.12	0.34	14.47
$[C_{12}H_{14}N]_2PbBr_4/MoSe_2$	1.23	1.48	0.95	0.23	18.02
$[C_{14}H_{18}NO]_2PbI_4/WSe_2$	1.24	1.42	0.85	0.27	17.29
$[C_7H_9FN]_2PbCl_4/WS_2$	1.25	1.93	1.60	0.03	16.10
$[C_6H_5CH_2NH_3]_2PbI_4/WS_2$	1.25	1.91	1.55	0.06	15.95
$[CH_3(CH_2)_3NH_3]_2PbI_4/MoS_2$	1.25	1.81	1.28	0.23	15.46
$[C_6H_5CH_2NH_3]_2PbBr_4/WS_2$	1.28	1.97	1.57	0.09	14.84
$[CH_3(CH_2)_5NH_3]_2PbI_4/MoS_2$	1.28	1.77	0.89	0.58	11.31
$[C_6H_{11}NH_3]_4Pb_2Cl_8/WS_2$	1.29	1.88	1.41	0.18	15.08
$[CH_3(CH_2)_3NH_3]_2CsPb_2Br_7/WS_2$	1.30	1.85	0.48	1.08	5.37
$[CH_3(CH_2)_3NH_3]_2PbI_4/WSTe$	1.30	2.15	1.73	0.12	11.92
$[CH_3(CH_2)_3NH_3]_2PbI_4/WSTe$	1.30	2.18	1.76	0.12	11.66
$[C_6H_{11}NH_3]_2PbBr_4/MoSSe$	1.30	1.68	1.21	0.17	17.45
$[C_7H_9FN]_2PbCl_4/MoSe_2$	1.31	1.43	1.11	0.02	22.43
$[I(CH_2)_4NH_3]_2PbI_4/WSSe$	1.32	1.72	1.28	0.13	17.69
$[CH_3(CH_2)_3NH_3]_2PbI_4/WSTe$	1.32	2.18	1.78	0.10	11.76
$[C_{14}H_{18}NO]_2PbI_4/WSSe$	1.34	1.52	0.88	0.35	15.72
$[I(CH_2)_6NH_3]_2PbI_4/WSe_2$	1.34	1.92	1.41	0.21	14.30
$[BrC_6H_4(CH_2)_2NH_3]_2PbI_4/WS_2$	1.35	1.57	0.71	0.56	11.89
$[C_5H_{10}F_2N]_2PbI_4/MoS_2$	1.37	1.79	1.48	0.01	18.40
$[C_5H_{10}F_2N]_2PbI_4/WSe_2$	1.38	2.02	1.65	0.07	14.28
$[C_6H_{11}NH_3]_2PbBr_4/MoSe_2$	1.39	1.53	1.02	0.22	17.97
$[C_6H_5CH_2NH_{3]2}SnBr_4/MoSSe$	1.23	1.44	0.22	0.03	22.11
$[C_6H_5CH_2NH_3]_2PbI_4/MoSSe$	1.40	1.65	1.33	0.02	20.07
$[C_6H_5CH_2NH_3]_2PbI_4/MoSe_2$	1.41	1.49	1.17	0.02	21.76
$(DFP)_2PbI_4/WSe_2$	1.41	1.94	1.63	0.01	16.11
$[C_6H_5CH_2NH_3]PbI_4/MoSe_2$	1.41	1.50	1.17	0.03	21.62
$[C_{14}H_{18}NO]_2PbI_4/MoSe_2$	1.42	1.48	1.16	0.02	21.85
$[CH_3(CH_2)_5NH_3]_2PbI_4/WSSe$	1.43	1.94	1.33	0.31	13.03
$[C_5H_{10}F_2N]_2PbI_4/WSSe$	1.44	1.75	1.21	0.24	15.91
$(BA)_2PbBr_4/WSe_2$	1.44	1.59	1.06	0.23	17.34
$[CH_3(CH_2)_5NH_3]_2PbI_4/MoSe_2$	1.45	1.91	1.55	0.06	15.92
$[CH_3(CH_2)_3NH_3]_2SnI_4/WSSe$	1.47	1.72	1.40	0.02	19.19
$[I(CH_2)_4NH_3]_2PbI_4/WSe_2$	1.48	1.65	1.21	0.14	18.40
$[CH_3(CH_2)_3NH_3]_2PbBr_4/WS_2$	1.49	1.88	0.61	0.97	6.55
$[I(CH_2)_5NH_3]_2PbI_4/WSe_2$	1.49	1.95	1.6	0.06	15.30
$[4\text{-}Cl\text{-}2\text{-}FBA]PbBr_4/MoS_2$	1.50	1.85	1.34	0.21	15.24
$(DFP)_2PbI_4/WSSe$	1.50	1.82	1.36	0.16	16.26
$[C_{12}H_{14}N]_2PbBr_4/WSe_2$	1.51	1.57	1.08	0.19	18.03
$[C_5H_5BrN]_2PbBr_4/MoSSe$	1.51	1.65	1.34	0.01	20.46
$[CH_3(CH_2)_3NH_3]_2PbBr_4/WS_2$	1.51	1.89	0.64	0.95	6.80
$(C_{13}H_{27}NH_3)_2PbI_4/WS_2$	1.53	1.91	1.58	0.03	16.38
$[I(CH_2)_5NH_3]_2PbI_4/WS_2$	1.55	1.93	1.56	0.07	15.55

$[CH_2CHCH_2NH_3]_2[CH_3CH_2NH_3]_2Pb_3Br_{10}$/MoSSe	1.55	1.57	0.97	0.31	16.18
$[C_6H_{11}NH_3]_4Pb_2Cl_8$/MoSSe	1.56	1.67	1.32	0.05	19.29
$[C_{12}H_{14}N]_2PbBr_4$/WSSe	1.56	1.77	1.43	0.04	18.21
$[C_8H_{11}FN]_2PbBr_4/MoS_2$	1.56	1.83	1.40	0.14	16.30
$[CH_3(CH_2)_3NH_3]_2CsPb_2Br_7$/MoSSe	1.57	1.68	1.05	0.33	15.15
$[I(CH_2)_6NH_3]_2PbI_4/MoS_2$	1.59	1.85	1.29	0.26	14.61
$[I(CH_2)_6NH_3]_2PbI_4$/WSSe	1.59	2.07	1.64	0.13	12.94
$[C_5H_5BrN]_2PbBr_4/WTe_2$	1.60	1.95	1.63	0.02	15.70
$[C_5H_5BrN]_2PbBr_4$/WSTe	1.60	1.86	1.19	0.37	13.21
$[C_7H_9FN]_2PbCl_4$/WSTe	1.60	2.80	2.42	0.08	3.99
$[C_7H_9FN]_2PbCl_4$/WSSe	1.60	1.95	1.63	0.02	15.76
$[CH_3(CH_2)_3NH_3]_2PbI_4/WS_2$	1.60	1.95	1.63	0.02	15.75
$[CH_3(CH_2)_3NH_3]_2PbI_4$/WSTe	1.61	1.94	1.55	0.09	15.20
$[CH_3(CH_2)_3NH_3]_2PbI_4/MoS_2$	1.61	1.94	1.61	0.03	15.85
$[CH_3(CH_2)_3NH_3]_2PbI_4/WS_2$	1.61	1.94	1.51	0.12	14.91
$[CH_3(CH_2)_3NH_3]_2PbI_4$/WSTe	1.61	1.94	1.55	0.09	15.23
$[CH_3(CH_2)_3NH_3]_2PbI_4/MoS_2$	1.61	1.93	1.59	0.04	15.92
$[_4$-Cl-$_2$-FBA$]PbBr_4/WS_2$	1.63	1.77	1.35	0.12	17.24
$[_4$-Cl-$_2$-FBA$]PbBr_4/MoS_2$	1.63	1.94	1.53	0.12	14.93
$[R-_4$-Cl-MBA$]_2PbBr_4$/WSSe	1.63	1.70	1.39	0.01	19.54
$(DFP)_2PbI_4/WS_2$	1.64	1.84	1.43	0.11	16.51
$(DFP)_2PbI_4/MoS_2$	1.65	1.91	1.59	0.02	16.33
$(DFP)_2PbI_4/WSe_2$	1.66	1.85	1.28	0.27	14.39
$(DFP)_2PbI_4$/WSSe	1.68	2.02	1.71	0.01	14.91
$(C_{11}H_{23}NH_3)_2PbI_4$/MoSSe	1.68	1.73	1.41	0.02	19.16
$(C_{11}H_{23}NH_3)_2PbI_4/MoS_2$	1.69	1.73	1.41	0.02	19.10
$(C_{13}H_{27}NH_3)_2PbI_4/WS_2$	1.69	1.73	1.41	0.02	19.06
$(C_{13}H_{27}NH_3)_2PbI_4$/MoSSe	1.75	1.89	1.47	0.12	15.57
$(C_{13}H_{27}NH_3)_2PbI_4/MoS_2$	1.87	1.94	1.57	0.07	15.52
$(C_{15}H_{31}NH_3)_2PbI_4/MoS_2$	1.88	1.94	1.37	0.28	13.32
$(C_{15}H_{31}NH_3)_2PbI_4/MoS_2$	1.90	1.93	1.47	0.16	14.68
$(BA)_2PbBr_4/WSe_2$	1.90	1.90	1.42	0.19	14.75
$[C_7H_9FN]_2PbCl_4$/MoSSe	1.37	1.65	1.34	0.01	20.39