First-principles guidelines to select promising van der Waals materials for hybrid photovoltaic-triboelectric nanogenerators — Electronic Supporting Information

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1 Bader charges

The charge variation $\delta\rho(Z)$ on an element Z occurring by changing the geometry setup is calculated as

$$\delta\rho(Z) = -(\rho_Y(Z) - \rho_0(Z)) \quad (1)$$

where ρ_0 is the charge calculated in the reference configuration (setup 0), while ρ_Y is the charge in the shifted configuration ($Y = A,B,C,D$). According to this definition, positive values of $\delta\rho(Z)$ indicate a loss of electrons, while negative values imply a gain of electrons. The $\delta\rho(Z)$ values calculated on all the systems are reported in Table 1 and Table 2, where "layer 1" and "layer 2" refer to the MX_2 layer attached to the left and right electrode, respectively.

Table 1 Charge variation $\delta\rho(Z)$ ($|e|$/unit cell) calculated on the Z part of the system ($Z =$ layer or electrode) for all the considered chemical compositions at different shifted Y configurations with $Y = A,B,C,D$.

MoS/CrS	Z	A	B	C	D
layer 1	MoS	0.14	0.09	-0.25	0.03
layer 2	CrS	0.23	-0.07	0.22	-0.02
electrode	right	-0.10	-0.03	0	0
electrode	left	-0.28	0	0.04	0
MoSe/WS	Z	A	B	C	D
layer 1	MoSe	-0.04	0.17	-0.65	0.17
layer 2	WS	0.25	-0.23	0.6	-0.17
electrode	right	-0.01	0.02	0.03	0
electrode	left	-0.21	0.01	0.02	-0.01
MoSe/WSe	Z	A	B	C	D
layer 1	MoSe	0.09	-0.19	-0.02	-0.02
layer 2	WSe	0	0.19	-0.01	0.02
electrode	right	-0.06	0.01	0	-0.01
electrode	left	-0.05	-0.03	0.02	0
MoSe/WTe	Z	A	B	C	D
layer 1	MoSe	0.21	-0.22	0.7	-0.22
layer 2	WTe	-0.37	0.22	-0.73	0.21
electrode	right	-0.1	-0.03	0.01	0
electrode	left	0.28	0	0.02	0.01
WS/PtS	Z	A	B	C	D
layer 1	WS	0.04	0.05	-0.46	0.04
layer 2	PtS	0.37	-0.04	0.44	-0.03
electrode	right	-0.08	-0.01	0	-0.01
electrode	left	-0.35	0	0.01	0
WS/RuS	Z	A	B	C	D
layer 1	WS	0.1	-0.1	-0.25	-0.04
layer 2	RuS	0.28	0.1	0.24	0.07
electrode	right	-0.06	-0.01	0	-0.02
electrode	left	-0.32	0.02	0.01	-0.01

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Table 2 Charge variation $\delta\rho(Z)$ ($|e|$/unit cell) calculated on the Z part of the system ($Z =$ layer or electrode) for all the considered chemical compositions at different shifted Y configurations with $Y = A, B, C, D$.

MoS/NiS	Z	A	B	C	D
layer 1	MoS	0.22	-0.11	-0.27	-0.03
layer 2	NiS	0.16	0.1	0.24	0.02
electrode	right	-0.06	0.02	0.01	0
electrode	left	-0.33	-0.02	0.02	0
MoS/PtS	Z	A	B	C	D
layer 1	MoS	0.13	0	-0.47	0.03
layer 2	PtS	0.23	0.02	0.45	-0.02
electrode	right	-0.05	0.01	0.01	0
electrode	left	-0.3	0	0.03	0
MoS/RuS	Z	A	B	C	D
layer 1	MoS	0.1	-0.14	-0.18	-0.06
layer 2	RuS	0.26	0.12	0.16	0.07
electrode	right	-0.05	0.02	0	-0.01
electrode	left	-0.3	0	0.02	0
MoS/WS	Z	A	B	C	D
layer 1	MoS	0.29	-0.02	0.14	0.01
layer 2	WS	0.18	0.02	-0.11	0.02
electrode	right	-0.19	0.02	0	-0.01
electrode	left	-0.27	-0.01	-0.01	0
MoTe/WSe	Z	A	B	C	D
layer 1	MoTe	0.05	0.17	-0.46	0.16
layer 2	WSe	0.09	-0.11	0.43	-0.17
electrode	right	0.01	-0.01	0.01	-0.01
electrode	left	-0.13	-0.05	0.01	0.01
MoTe/WTe	Z	A	B	C	D
layer 1	MoTe	0.1	-0.01	0.05	-0.02
layer 2	WTe	-0.15	-0.01	-0.07	0.01
electrode	right	-0.06	0	0	0
electrode	left	0.11	0	0.01	0.01
WS/CrS	Z	A	B	C	D
layer 1	WS	0.11	0.19	-0.29	0.04
layer 2	CrS	-1.31	-0.2	0.24	-0.04
electrode	right	-0.08	-0.04	0.03	0
electrode	left	1.27	0.03	0.02	0
WS/NiS	Z	A	B	C	D
layer 1	WS	0.08	-0.08	-0.33	-0.05
layer 2	NiS	0.29	0.07	0.31	0.07
electrode	right	-0.07	0	0.02	-0.01
electrode	left	-0.3	0.01	0.03	0