Superconductivity in Janus M_2X MXenes (M = W, Mo, Nb, and X = C, N) functionalized with hydrogen and bromine

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Tables S1 and S2 summarize the adsorption site configurations of Janus MXenes in the 1T and 2H phases, respectively. Tables S3–S8 report the calculated total energies (Etot) and formation energies (Δ_E) for all configurations of Mo_2CHBr, Mo_2NHBr, W_2CHBr, W_2NHBr, Nb_2CHBr, and Nb_2NHBr.

Table S1. 1T-phase Janus MXene adsorption site configurations.

Config.	Hydrogen Site	Bromine Site	Atomic Position Description
1	Top-M_2	Top-M_2	Both above **M_2** transition metal
2	Hollow	Hollow	Both at **hexagon center**
3	Top-M_2	Hollow	H above M_2, Br at hexagon center
4	Hollow	Top-M_2	H at hexagon center, Br above M_2
5	Top-M_1	Top-M_1	Both above **M_1** transition metal
6	Top-M_1	Top-M_2	H above M_1, Br above M_2
7	Top-M_2	Top-M_1	H above M_2, Br above M_1
8	Hollow	Top-M_1	H at hexagon center, Br above M_1
9	Top-M_1	Hollow	H above M_1, Br at hexagon center

Table S2. 2H-phase Janus MXene configurations.

Config.	Hydrogen Site	Bromine Site	Atomic Arrangement
1	Top-M	Top-M	Both above transition metals
2	Top-X	Top-X	Both above X atoms
3	**Hollow**	**Hollow**	Both at hexagon centers
4	**Hollow**	Top-X	H at hexagon center, Br above X
5	Top-X	**Hollow**	H above X, Br at hexagon center
6	Top-X	Top-M	H above X, Br above M
7	Top-M	Top-X	H above M, Br above X
8	Top-M	**Hollow**	H above M, Br at hexagon center
9	**Hollow**	Top-M	H at hexagon center, Br above M

Table S3. The total energy (Etot) of Mo_2CHBr structures along with their formation energy (Δ_E) is presented for each configuration.

1T	$\Delta_E(eV)$	2H	$\Delta_E(eV)$
S1	-0.02	S1	0.42
S2	0.02	S2	0.09
S3	-0.03	S3	0.01
S4	0.05	S4	0.02
S5	0.12	S5	0.06
S6	0.05	S6	0.13
S7	0.00	S7	0.30
S8	0.03	S8	0.31
S9	0.07	S9	0.08

Table S4. The total energy (Etot) of Mo_2NHBr structures along with their formation energy (Δ_E) is presented for each configuration.

1T	$\Delta_E(eV)$	2H	$\Delta_E(eV)$
S1	-0.01	S1	0.18
S2	0.06	S2	0.02
S3	-0.02	S3	-0.11
S4	0.01	S4	-0.08
S5	0.08	S5	-0.04
S6	0.02	S6	0.03
S7	0.01	S7	0.16
S8	0.05	S8	0.14
S9	0.06	S9	-0.03

Table S5. The total energy (Etot) of W_2CHBr structures along with their formation energy (Δ_E) is presented for each configuration.

1T	$\Delta_E(eV)$	2H	$\Delta_E(eV)$
S1	0.21	S1	0.45
S2	0.24	S2	0.23
S3	0.19	S3	0.17
S4	0.27	S4	0.18
S5	0.21	S5	0.21
S6	0.21	S6	0.24
S7	0.17	S7	0.38
S8	0.21	S8	0.39
S9	0.22	S9	0.57

Table S6. The total energy (Etot) of W_2NHBr structures along with their formation energy (Δ_E) is presented for each configuration.

1T	$\Delta_E(eV)$	2H	$\Delta_E(eV)$
S1	0.08	S1	0.12
S2	0.19	S2	0.03
S3	0.12	S3	0.08
S4	0.14	S4	0.01
S5	0.12	S5	0.03
S6	0.14	S6	0.07
S7	0.06	S7	0.18
S8	0.09	S8	0.13
S9	0.14	S9	-0.02

Table S7. The total energy (Etot) of Nb_2CHBr structures along with their formation energy (Δ_E) is presented for each configuration.

1T	$\Delta_E(eV)$	2H	$\Delta_E(eV)$
S1	-0.58	S1	0.26
S2	-0.48	S2	-0.38
S3	-0.49	S3	-0.36
S4	-0.55	S4	-0.42
S5	-0.15	S5	-0.32
S6	-0.36	S6	-0.12
S7	-0.43	S7	-0.01
S8	-0.21	S8	0.03
S9	-0.27	S9	-0.17

Table S8. The total energy (Etot) of Nb_2NHBr structures along with their formation energy ($_{\Delta E}$) is presented for each configuration.

1T	$\Delta_E(eV)$	2H	$\Delta_E(eV)$
S1	-0.68	S1	-0.06
S2	-0.63	S2	-0.56
S3	-0.56	S3	-0.62
S4	-0.55	S4	-0.62
S5	-0.29	S5	-0.56
S6	-0.47	S6	-0.38
S7	-0.53	S7	-0.29
S8	-0.44	S8	-0.27
S9	-0.38	S9	-0.43

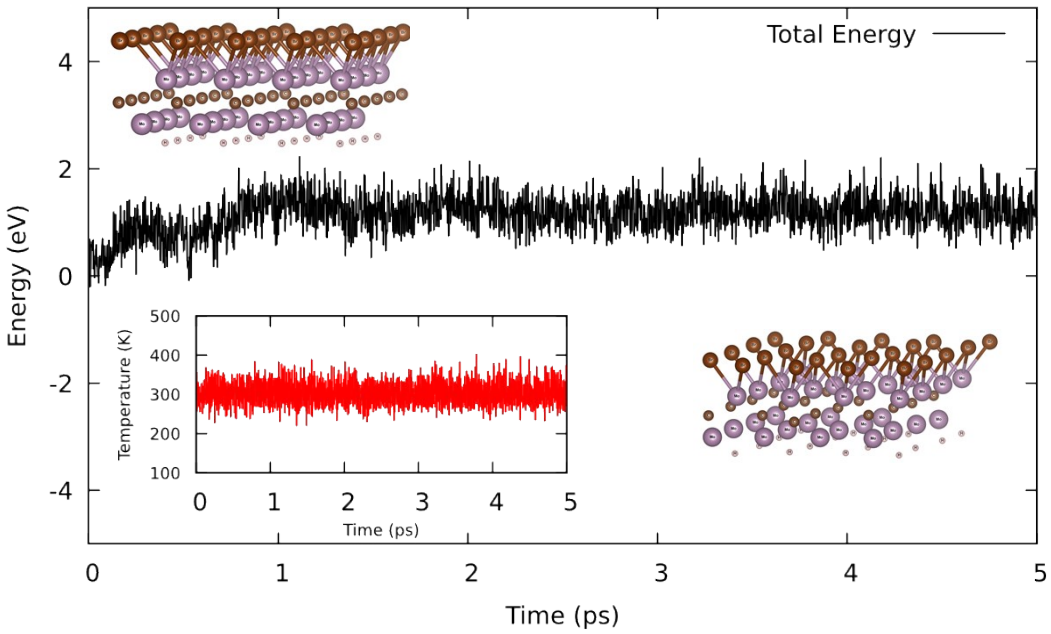

Figure S1. ab initio molecular dynamics (AIMD) simulations for a representative structure: the Mo_2CHBr Janus compound.

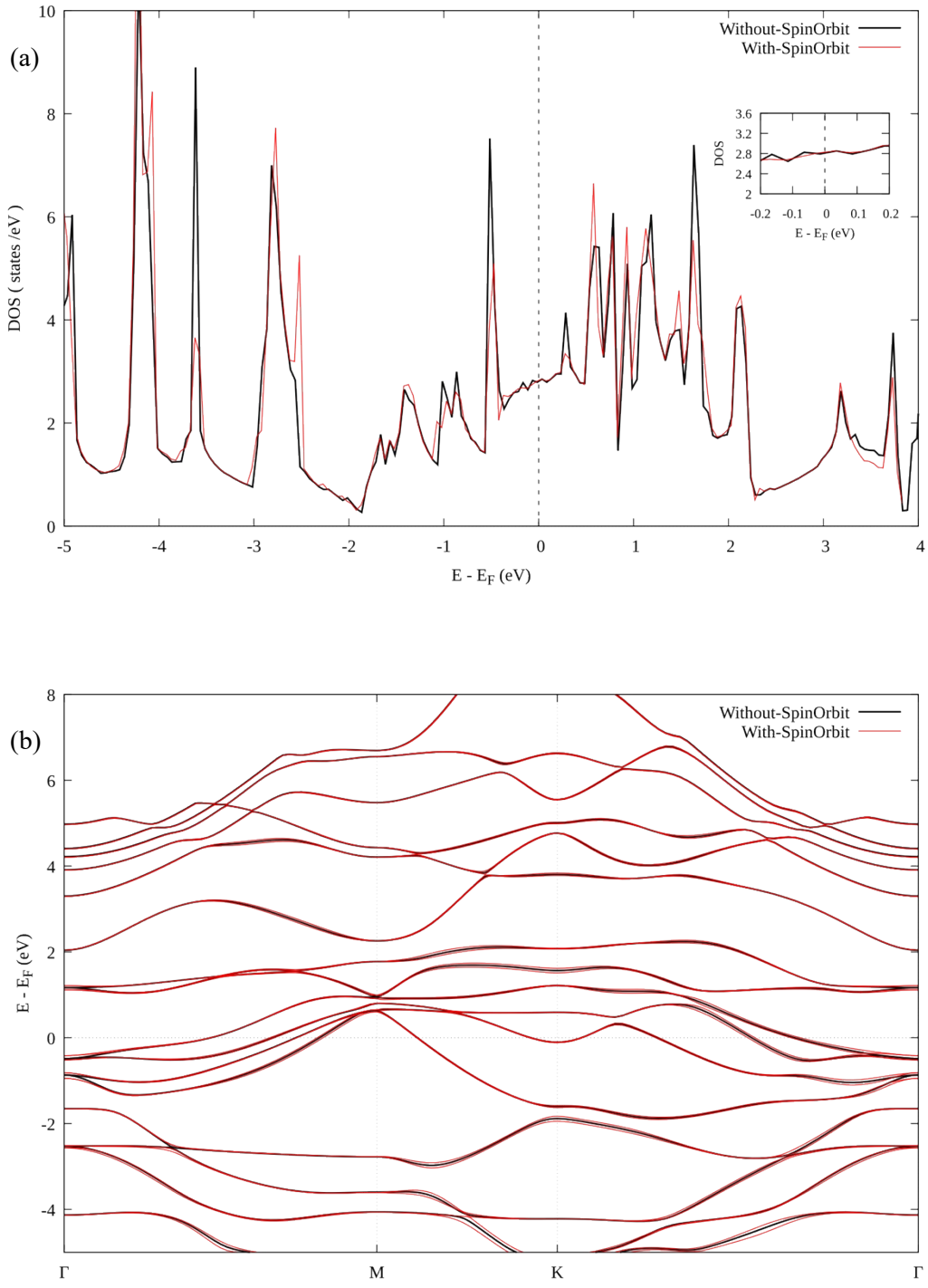

Figure S2. Density of states (a) and band structure (b) of the Mo_2CHBr compound, calculated with (red lines) and without (black lines) spin-orbit interaction.

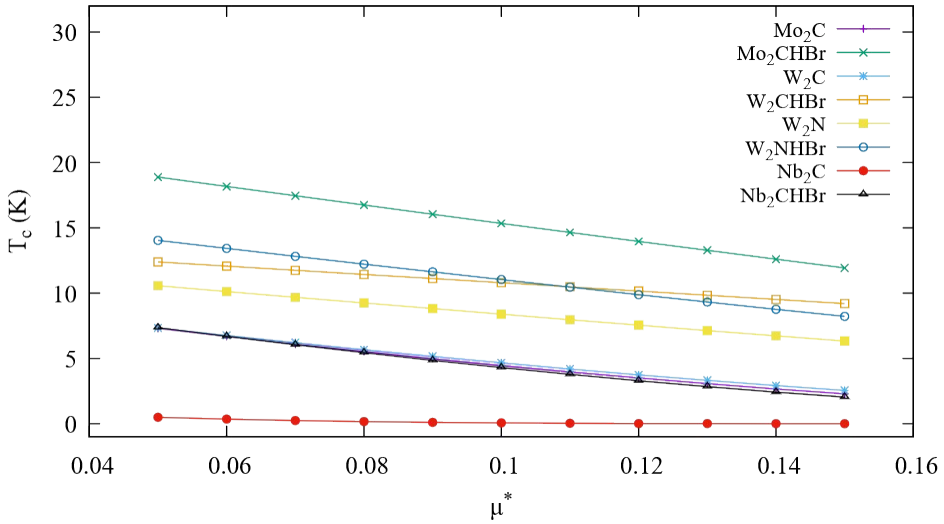

Figure S3. Dependence of the transition temperature on the Coulomb pseudopotential parameter (μ^*) for different compounds.