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Supplementary Information for:

Predicting Stable Phase Monolayer Mo_2C (MXene), a Superconductor with Chemically-Tunable Critical Temperature

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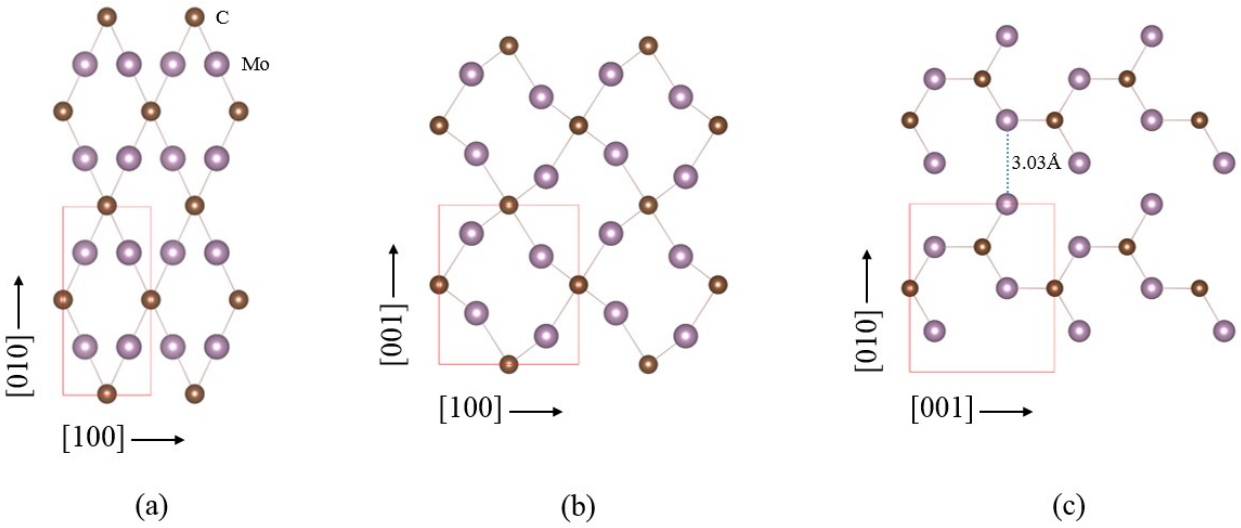

Fig. S1 Geometries of monolayer Mo_2C obtained by truncating bulk alpha-Mo_2C: (a) normal to [001] direction, (b) normal to [010] direction, and (**c**) normal to [100] direction. The red solid

lines exhibit the unit cells. Structure (a) is lower in energy by 0.3 eV with respect to (b). Mo atoms are not bonded in (**c**).

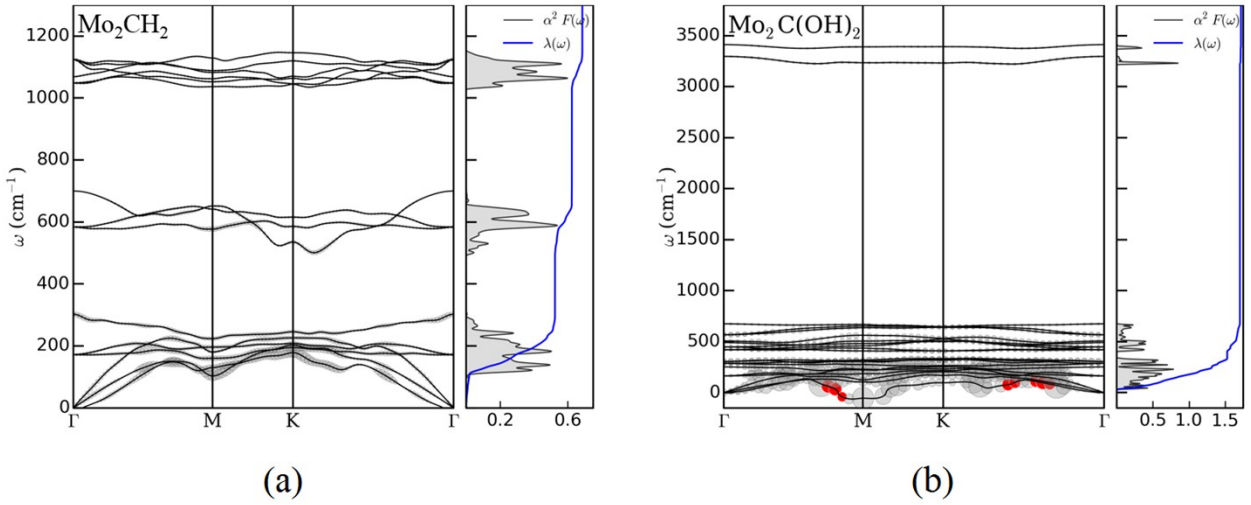

Fig. S2 Phonon dispersions, electron-phonon interactions, Eliashberg spectral function, and the frequency-dependent electron-phonon couplings of (a) Mo_2CH_2, and (b) $Mo_2C(OH)_2$. Here, the q-mesh of 21×21×1 was used for both structures.

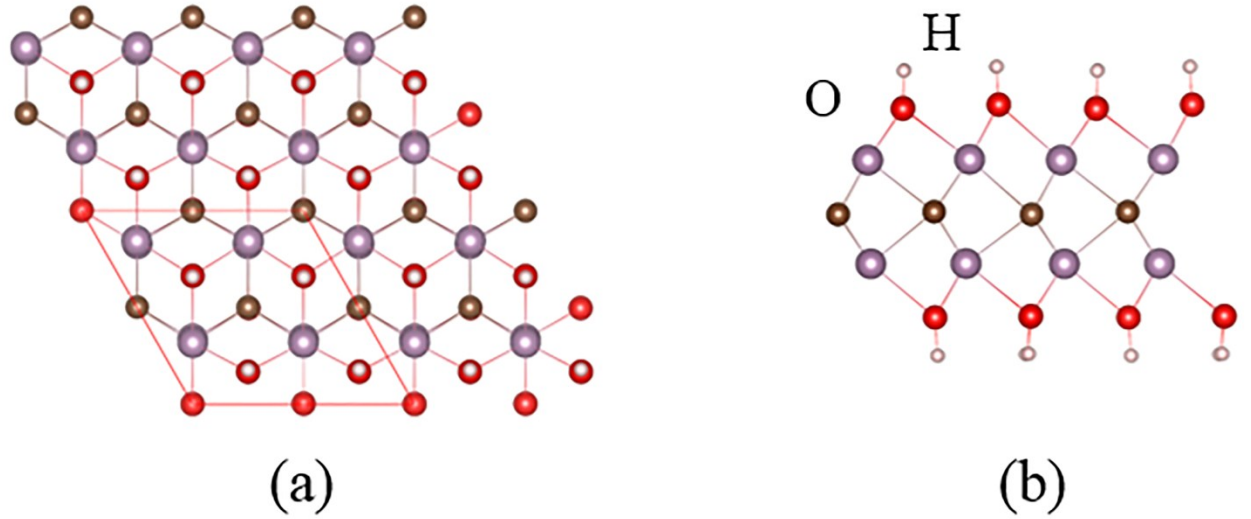

Fig. S3 Optimized geometry of the 2×2 $Mo_2C(OH)_2$ superstructure: (a) top, and (b) side views. This structure exhibits buckling.

Preliminary results for Ti_2C MXene

We have performed additional calculations of T_c in single-layer 1T Ti_2C and Ti_2CH_2. According to our analysis, the most stable phase for both is 1T. We further obtain a low T_c ~1.3 K in Ti_2C, predicting a transition in the sub-Kelvin regime, but not above the liquid He, 4.21 K. Such low T_c is seen to be due to weak electron-phonon coupling (the obtained e-ph coupling constant is λ~0.40). In Ti_2CH_2, the obtained T_c = 0 K, stemming from the extremely small e-ph coupling constant λ~0.13. In contrast, in bare Mo_2C, the e-ph coupling constant is λ~0.50, higher by 20%, yielding a T_c of 3.2 K, while in Mo_2CH_2 we had almost double value of λ~0.73 (ω_{ln} ~327 K), yielding a T_c of 12.6 K. Regarding surface termination dependence, surfaces of Ti_2C sheets are chemically active and are normally terminated with F, O and OH. However, O- and OH-terminated MXenes are most stable; moreover, at high temperatures, OH groups are converted into O terminations.[1] For this reason, O-termination would be most common in experiments. Unlike metallic Mo_2CO_2, Ti_2CO_2 is a semiconductor,[2] potentially preventing measuring superconductivity in this family of materials.

Table S1. Convergence test for Mo_2C MXene.

k-grid	**q**- grid	ω_{ln} [K]	λ	T_c [K]
21×21	21×21	192.151	0.53594	3.033
63×63	63×63	179.701	0.55554	3.213

Table S2. Convergence test for Mo_2CO_2 MXene.

k- grid	**q**- grid	ω_{ln} [K]	λ	T_c [K]
21×21	21×21	288.195	0.23567	0.006
63×63	63×63	299.649	0.23134	0.004

Table S3. Convergence test for Mo_2CH_2 MXene.

k- grid	**q**- grid	ω_{ln} [K]	λ	T_c [K]
21×21	21×21	329.806	0.68663	10.936
63×63	63×63	326.543	0.73205	12.626

Table S4. Convergence test for $Mo_2C(OH)_2$ MXene.

k- grid	**q**- grid	ω_{ln} [K]	λ	T_c [K]
21×21	21×21	198.947	1.71780	25.545
63×63	63×63	169.780	1.92960	23.817

Table S5. Convergence test for Ti_2C MXene.

k-grid	**q**- grid	ω_{ln} [K]	λ	T_c [K]
21×21	7×7	308.050	0.39861	1.268
21×21	21×21	305.756	0.40220	1.324

Table S6. Convergence test for Ti_2CH_2 MXene.

k-grid	**q**- grid	ω_{ln} [K]	λ	T_c [K]
21×21	7×7	540.798	0.13062	0.000
21×21	21×21	530.139	0.12895	0.000

References

1. Y. Xie, M. Naguib, V. N. Mochalin, M. W. Barsoum, Y. Gogotsi, X. Yu, K. W. Nam, X. Q. Yang, A. I. Kolesnikov and P. R. Kent, *J. Am. Chem. Soc.*, 2014, **136**, 6385-6394.
2. X.-f. Yu, J.-b. Cheng, Z.-b. Liu, Q.-z. Li, W.-z. Li, X. Yang and B. Xiao, *RSC Adv.*, 2015, **5**, 30438-30444.