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Theoretical assessment of Raman spectra on MXene Ti_2C: from monolayer to bilayer

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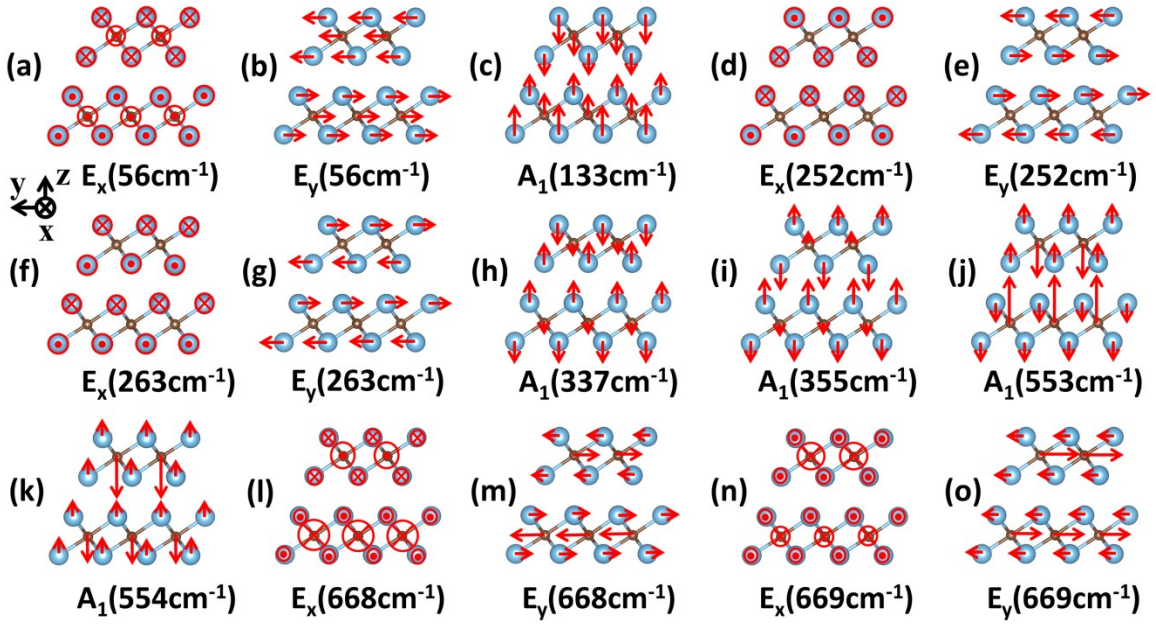

Figure S1. Atomic displacements of the Raman-active modes of bilayer Ti_2C. The optical modes with the same irreducible representation are labeled according to their frequencies. The cross (dot) on the atom corresponds to vibration direction pointing into (out of) the plane, and the arrow corresponds to the in-plane vibration. The in-plane (out-of-plane) vibration amplitude is illustrated by the length (size) of the arrow (circle).

Table SI. Raman tensor elements a, b, c and d for monolayer Ti_2C.

Wave Length	532nm	633nm
a(a.u.)	$14e^{(i\times41^\circ)}$	$48e^{(i\times84^\circ)}$
b(a.u.)	$74\ e^{(i\times13^\circ)}$	$11\ e^{(-i\times70^\circ)}$
c(a.u.)	$24e^{(i\times2^\circ)}$	$172e^{(-i\times23^\circ)}$
d(a.u.)	$46e^{(i\times38^\circ)}$	$40e^{(-i\times22^\circ)}$

Table SII. Raman tensor elements e, f, g and h for bilayer Ti_2C.

Mode	$A_1(133cm^{-1})$		$A_1(337cm^{-1})$		$A_1(355cm^{-1})$		$A_1(553cm^{-1})$		$A_1(554cm^{-1})$	
Wave Length	532nm	633nm	532nm	633nm	532nm	633nm	532nm	633nm	532nm	633nm
e(a.u.)	$45e^{(i\times80^\circ)}$	$122e^{(i\times86^\circ)}$	$35e^{(i\times11^\circ)}$	$110e^{(-i\times22^\circ)}$	$28e^{(i\times21^\circ)}$	$46e^{(i\times76^\circ)}$	$33e^{(i\times49^\circ)}$	$10e^{(-i\times15^\circ)}$	$115e^{(i\times52^\circ)}$	$51e^{(-i\times29^\circ)}$
f(a.u.)	$34e^{(i\times48^\circ)}$	$26e^{(i\times51^\circ)}$	$35e^{(i\times31^\circ)}$	$140e^{(i\times36^\circ)}$	$68e^{(i\times51^\circ)}$	$63e^{(i\times35^\circ)}$	$20e^{(-i\times20^\circ)}$	$111e^{(i\times62^\circ)}$	$67e^{(-i\times25^\circ)}$	$407e^{(i\times60^\circ)}$
Mode	$E(56cm^{-1})$		$E(252cm^{-1})$		$E(263cm^{-1})$		$E(668cm^{-1})$		$E(669cm^{-1})$	
Wave Length	532nm	633nm	532nm	633nm	532nm	633nm	532nm	633nm	532nm	633nm
g(a.u.)	$43e^{(-i\times17^\circ)}$	$94e^{(-i\times88^\circ)}$	$31e^{(i\times44^\circ)}$	$70e^{(-i\times57^\circ)}$	$92e^{(i\times48^\circ)}$	$173e^{(-i\times49^\circ)}$	$171e^{(-i\times84^\circ)}$	$98e^{(i\times48^\circ)}$	$96e^{(-i\times84^\circ)}$	$53e^{(i\times49^\circ)}$
h(a.u.)	$27e^{(-i\times67^\circ)}$	$147e^{(i\times51^\circ)}$	$56e^{(i\times29^\circ)}$	$126e^{(-i\times26^\circ)}$	$14e^{(i\times26^\circ)}$	$29e^{(-i\times34^\circ)}$	$28e^{(i\times21^\circ)}$	$56e^{(-i\times79^\circ)}$	$14e^{(i\times66^\circ)}$	$28e^{(-i\times69^\circ)}$