MXene Nanoribbons

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Here are the supplementary tables and figures:

TABLE S1. Calculated E_b (in eV), E_f (in eV), γ (in eV/Å), ΔE (in eV) and M (in μ_B) of F-functionalized Ti_2C nanoribbons.

		F-				
		E_b	E_f	γ	ΔE	M
zigzag	6-CTiTi-TiTiC	6.32	1.87	0.54	-0.01	0.01
	7-CTiTi-TiCTi	6.22	1.84	0.72	-0.17	-0.01
	8-CTiTi-CTiTi	6.23	1.94	0.54	-0.01	-0.01
	7-TiTiC-TiCTi	6.11	1.92	0.10	-0.19	1.43
	8-TiTiC-CTiTi	6.14	2.02	-0.44	-0.01	-0.11
	6-TiCTi-TiCTi	6.09	1.80	0.93	-0.31	1.72
armchair	6-ATi_2CNR	6.25	1.96	1.07	0.00	0.00
	7-ATi_2CNR	6.18	1.89	1.39	-0.12	1.16

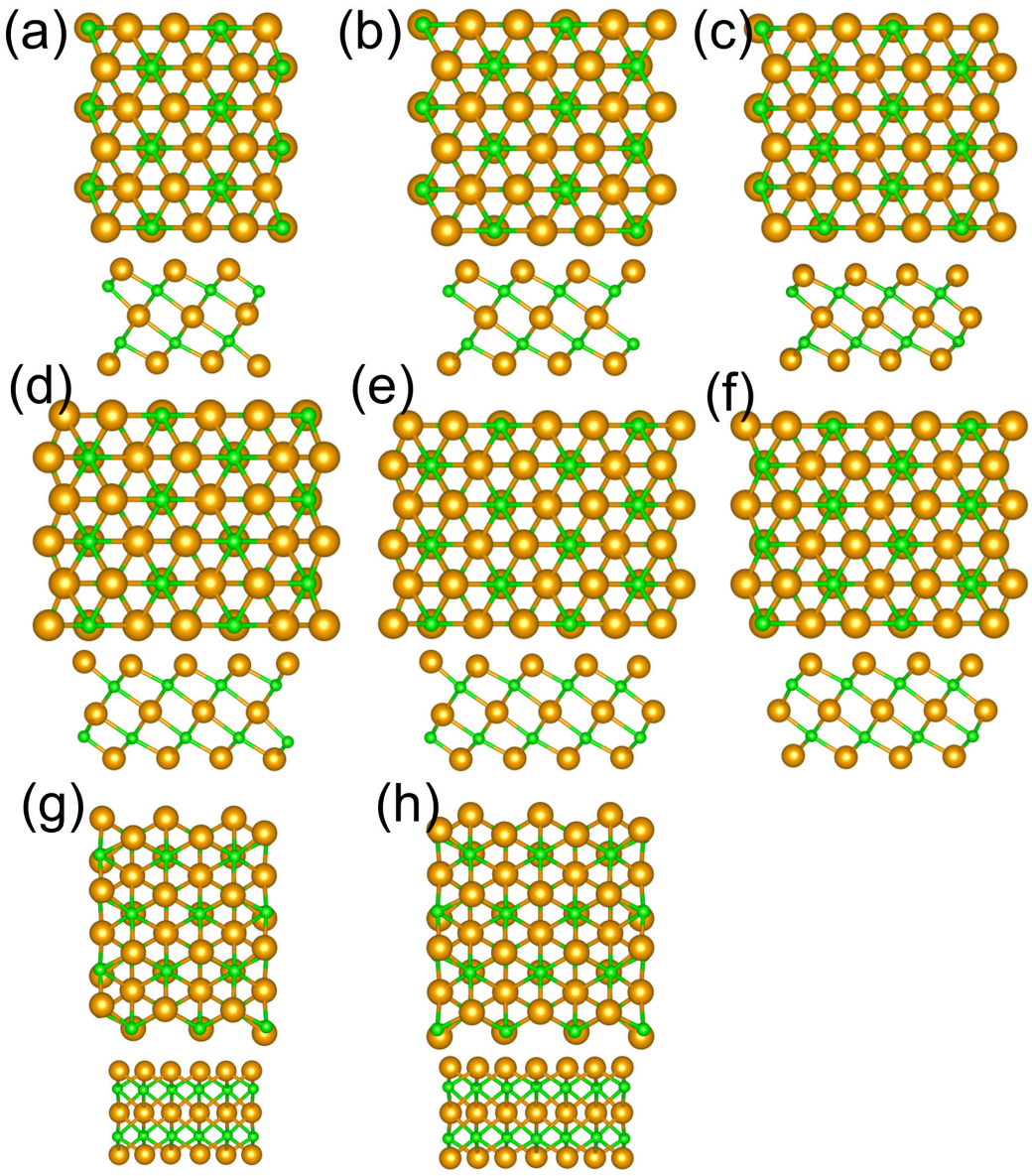

FIG. S1. Top view and side view of atomic configurations of Ti_3C_2 nanoribbons studied in this work.

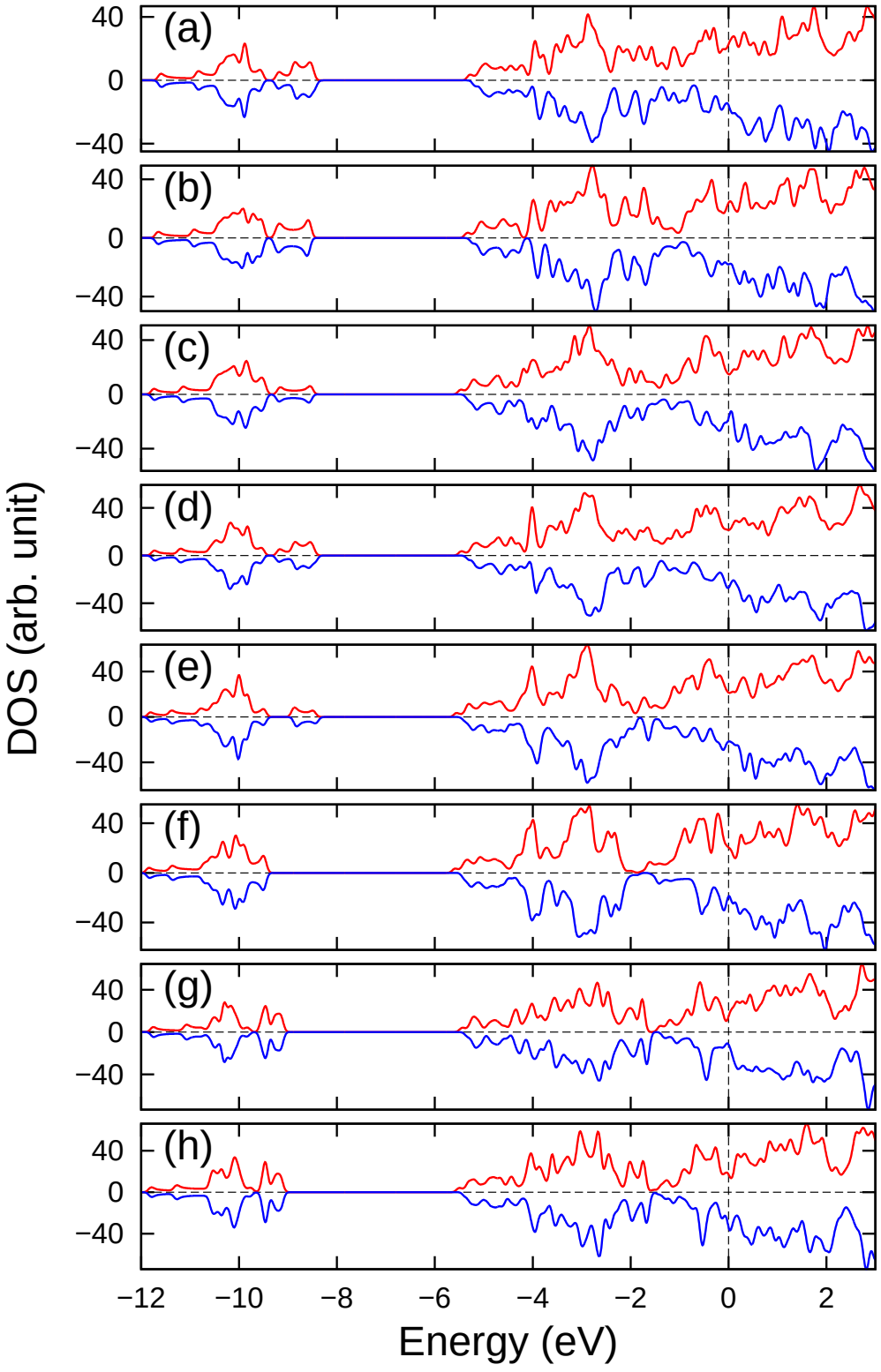

FIG. S2. Total density of states (DOS) of Ti_3C_2 nanoribbons. The sequence is the same as the structures shown in Fig. S1.

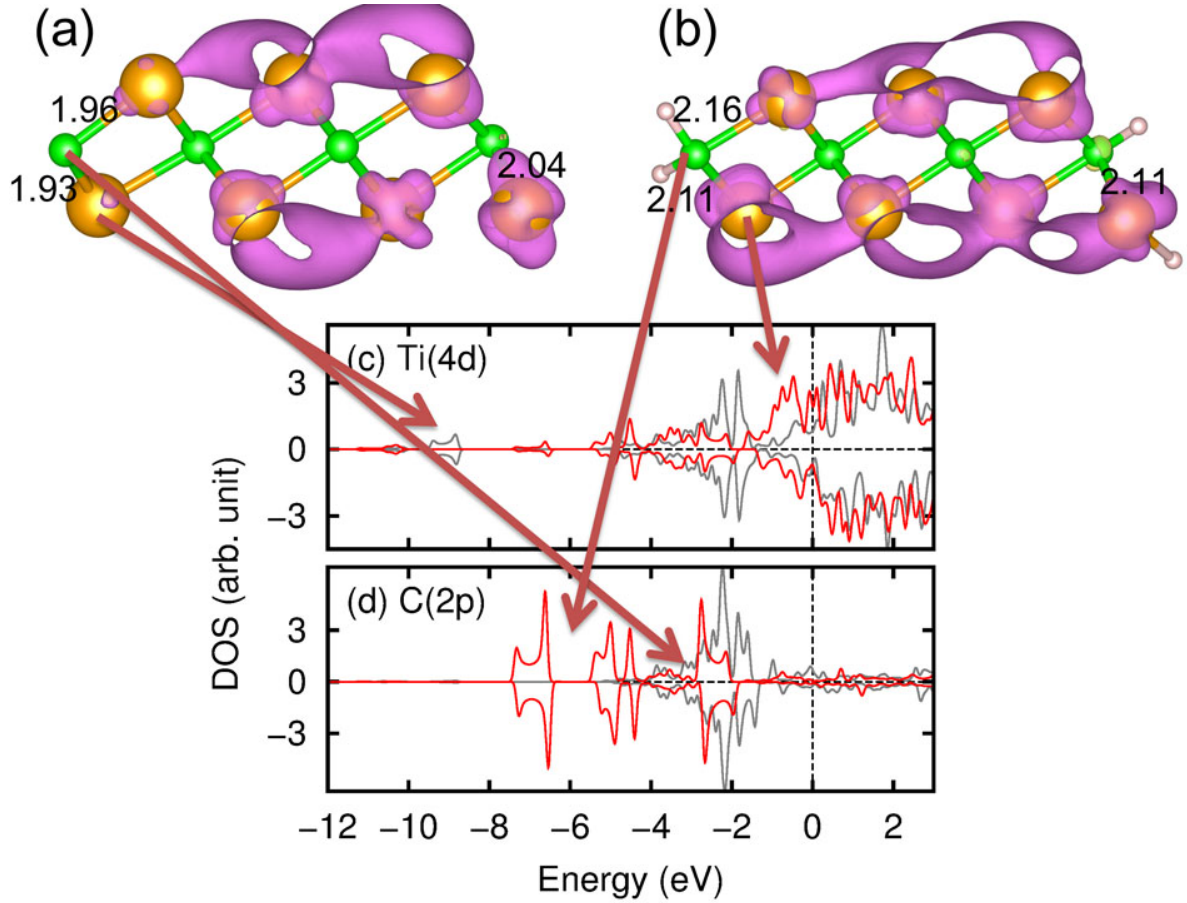

FIG. S3. Spin density plots of bare and hydrogen-passivated 7-CTiTi-TiCTi nanoribbons. The isovalue is ± 0.005 e^-/au^3 with positive represented by purple and negative by gold color. Some bonding distances are denoted in angstrom. The projected density of states (PDOS) of two edge atoms are provided below and the gray and red curves represent the PDOS of edge atoms in bare and hydrogen-passivated nanoribbons, respectively.

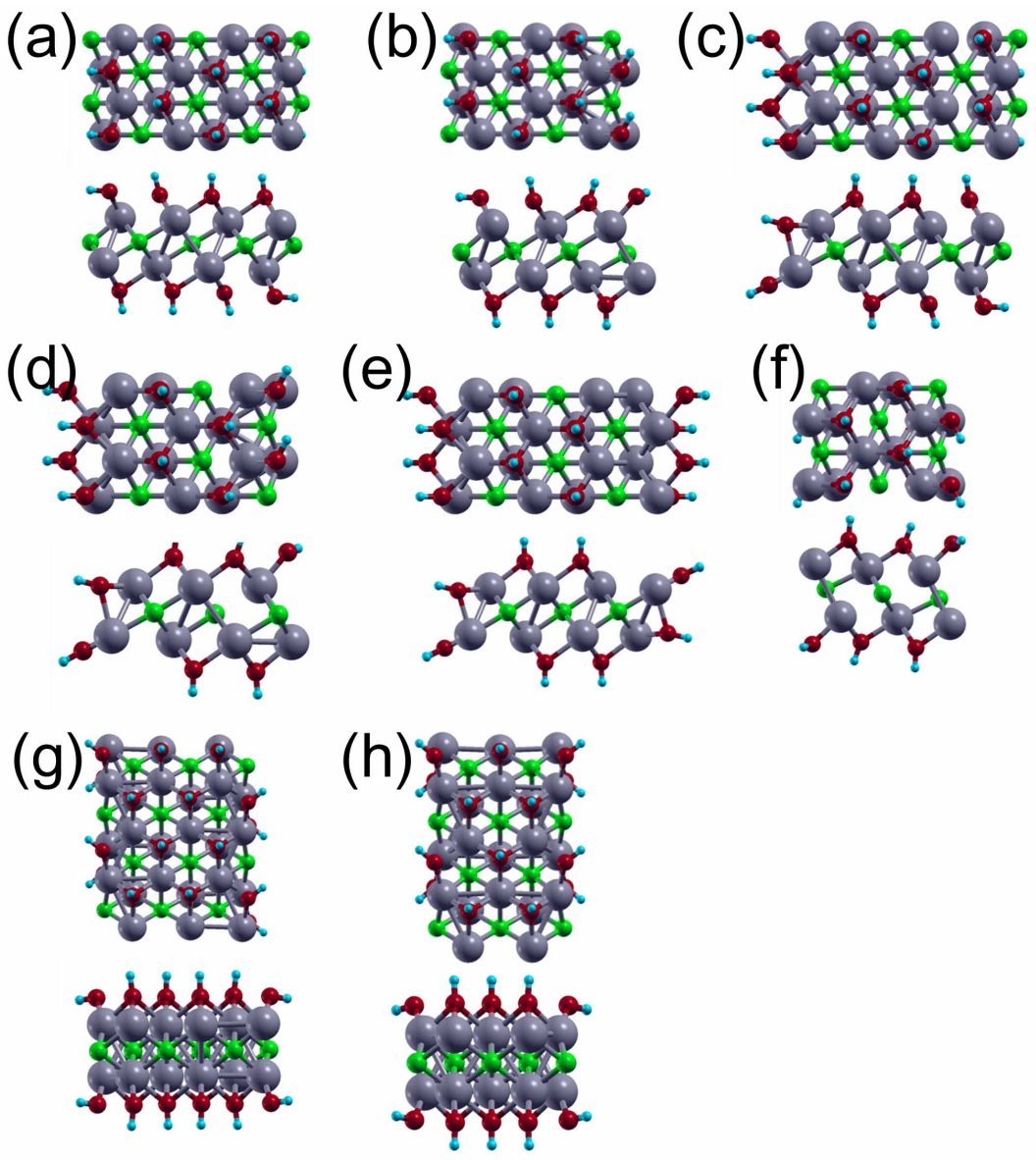

FIG. S4. Atomic configurations of $Ti_2C(OH)_2$ nanoribbons considered in this work.

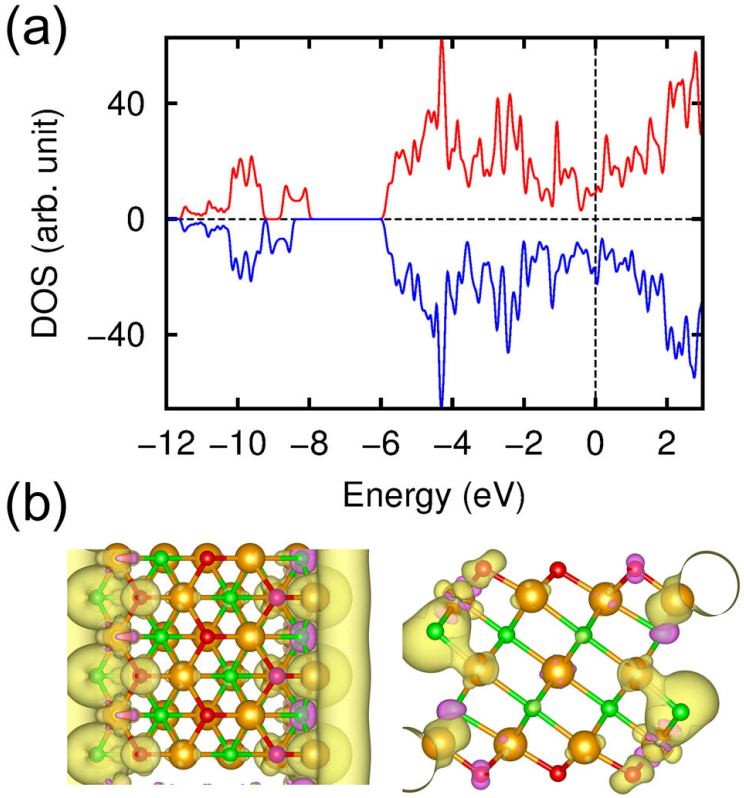

FIG. S5. (a) Total density of states of $Ti_3C_2O_2$ nanoribbons with the CTiTi-TiCTi type. The spin density isosurface plot is given in (b) with the isovalue of ± 0.005 e^-/au^3 with positive represented by purple and negative by gold color.

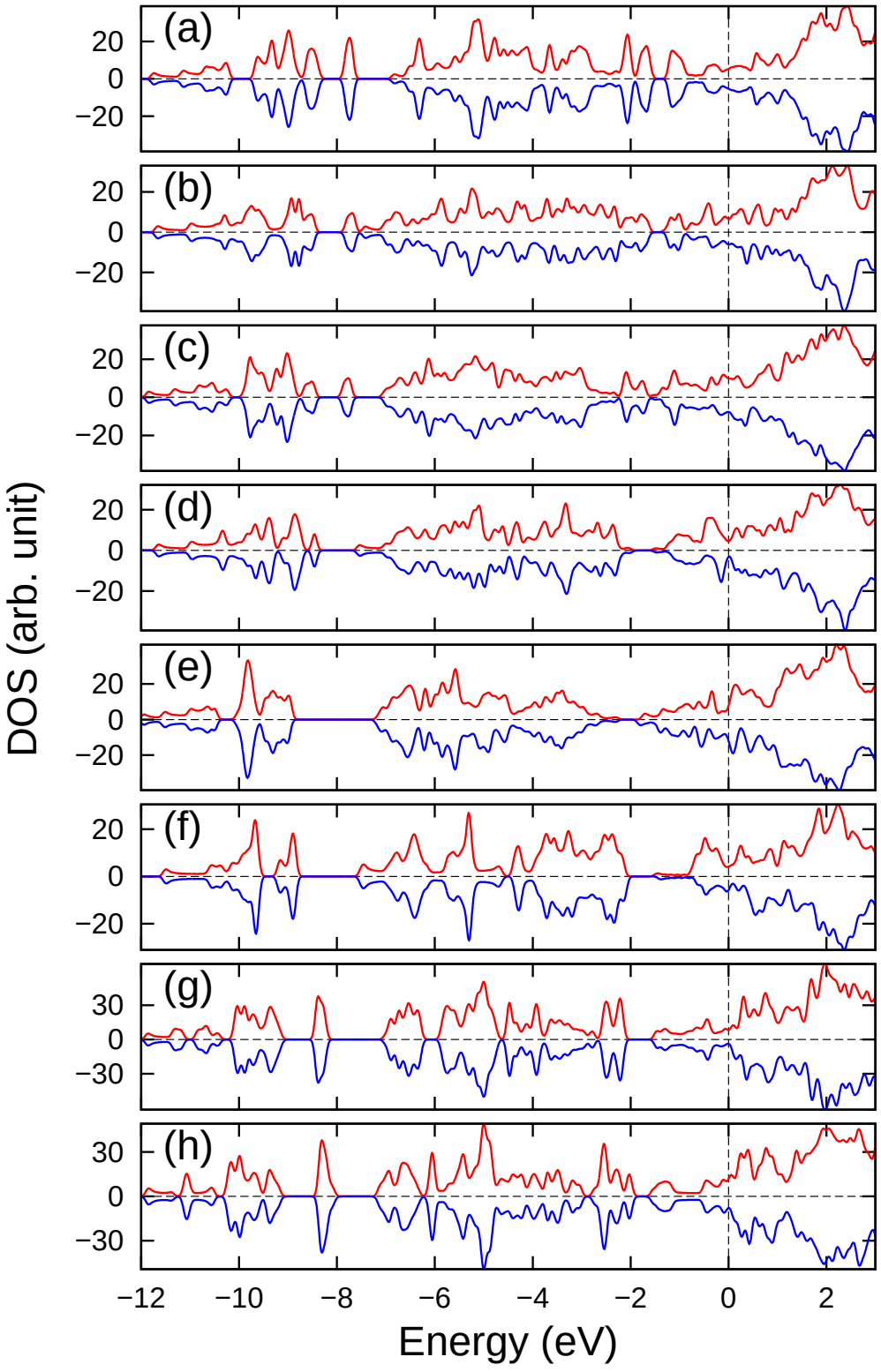

FIG. S6. Total density of states (DOS) of $Ti_3C_2(OH)_2$ nanoribbons. The sequence is the same as the structures shown in Fig. S4.

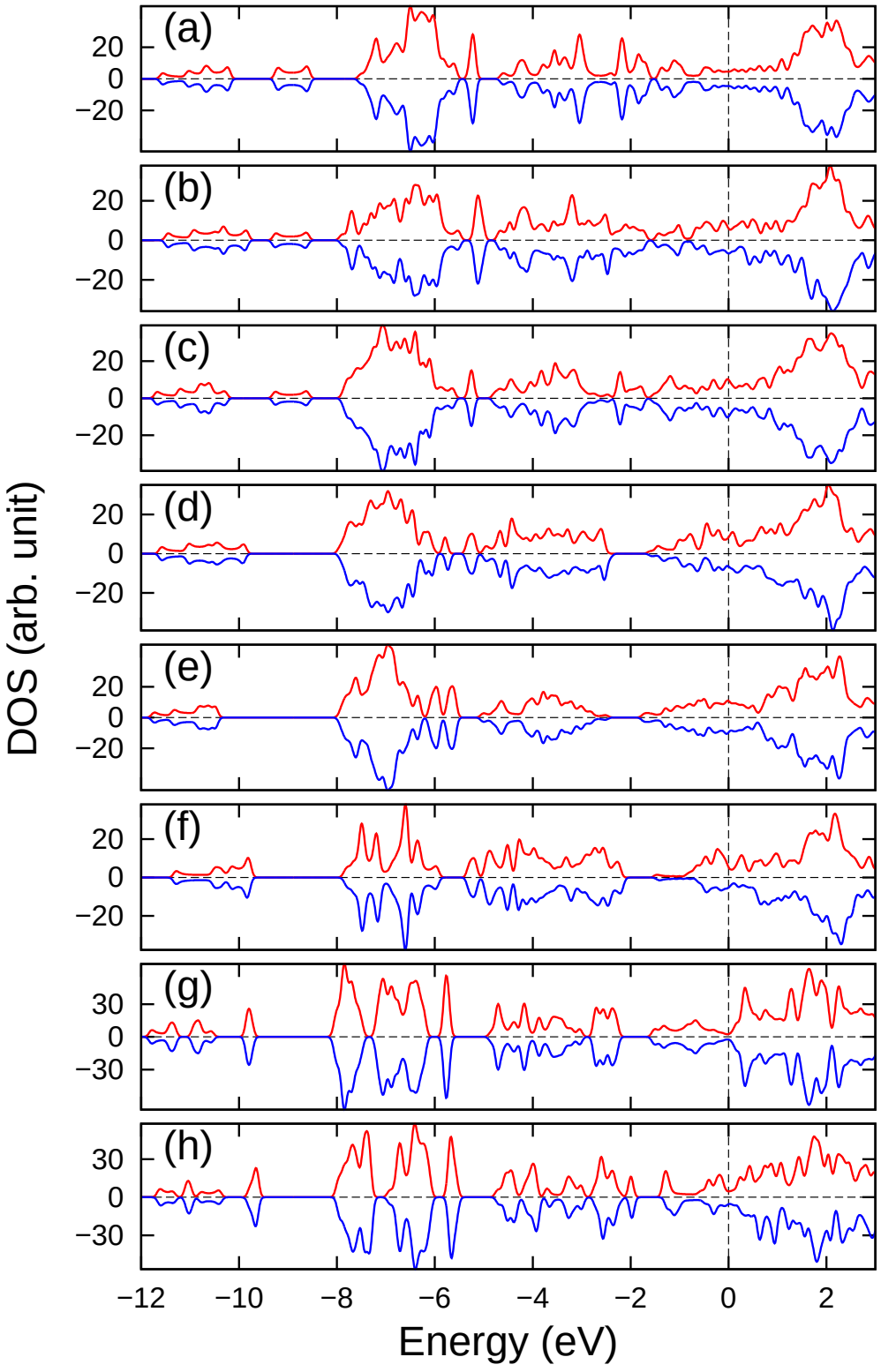

FIG. S7. Total density of states (DOS) of $Ti_3C_2F_2$ nanoribbons.

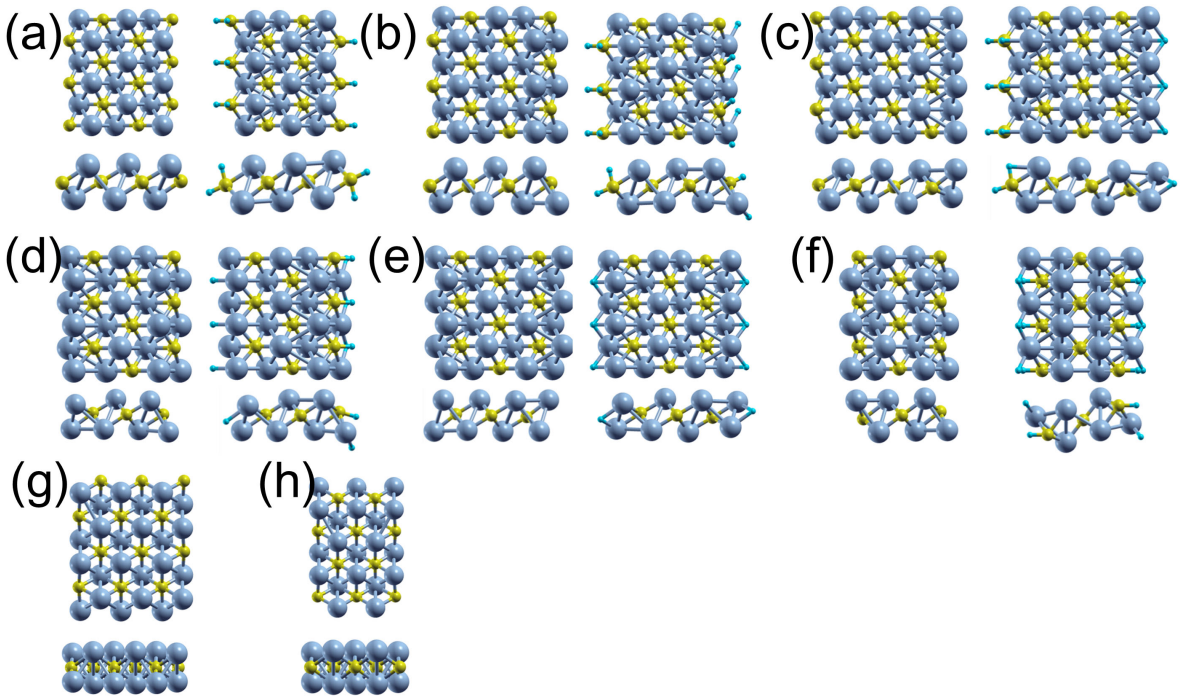

FIG. S8. Atomic configurations of pristine V_2C and corresponding H-passivated V_2C nanoribbons considered in this work.

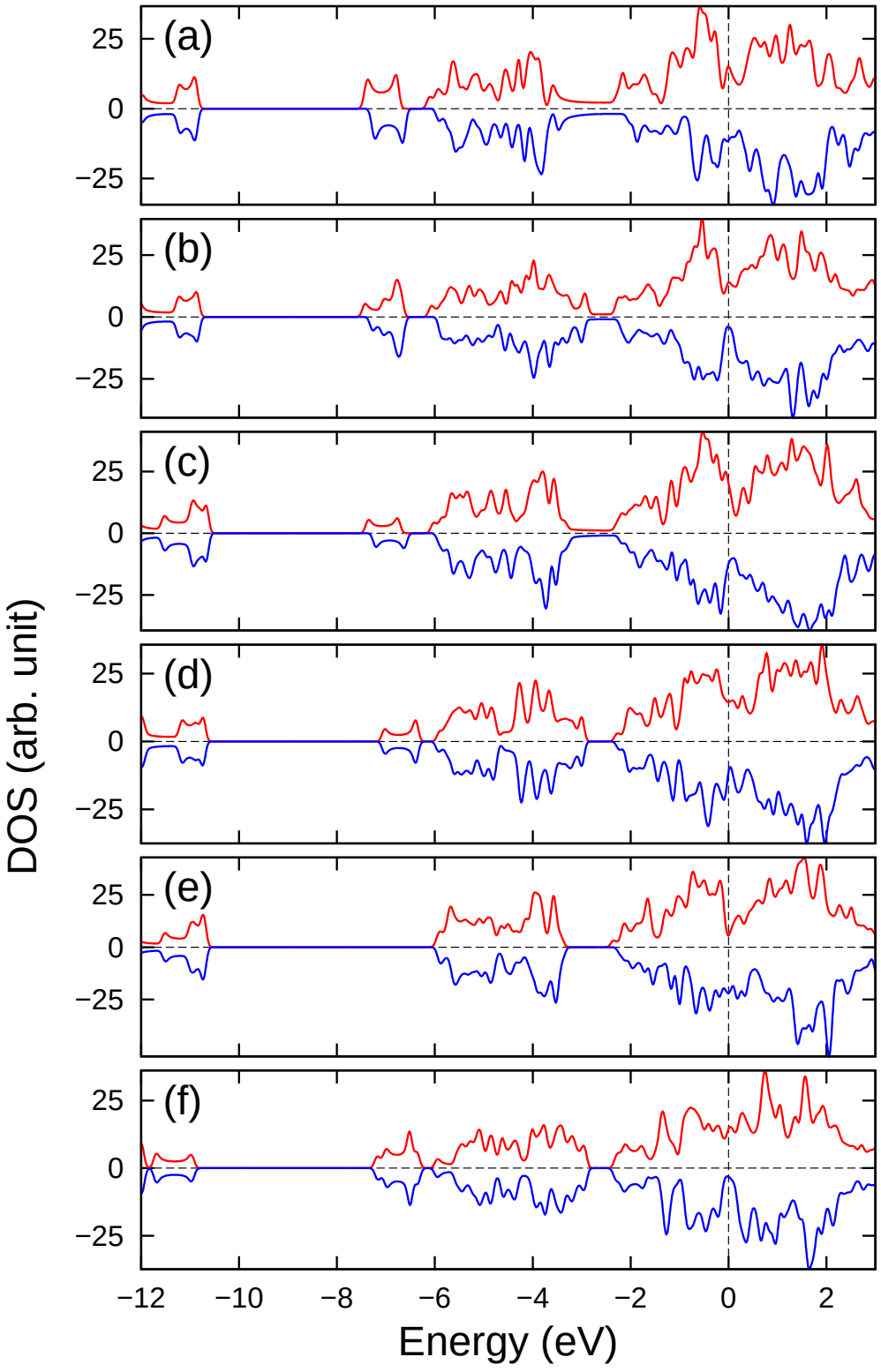

FIG. S9. Total density of states of hydrogen-passivated six types of zigzag V_2C nanoribbons.

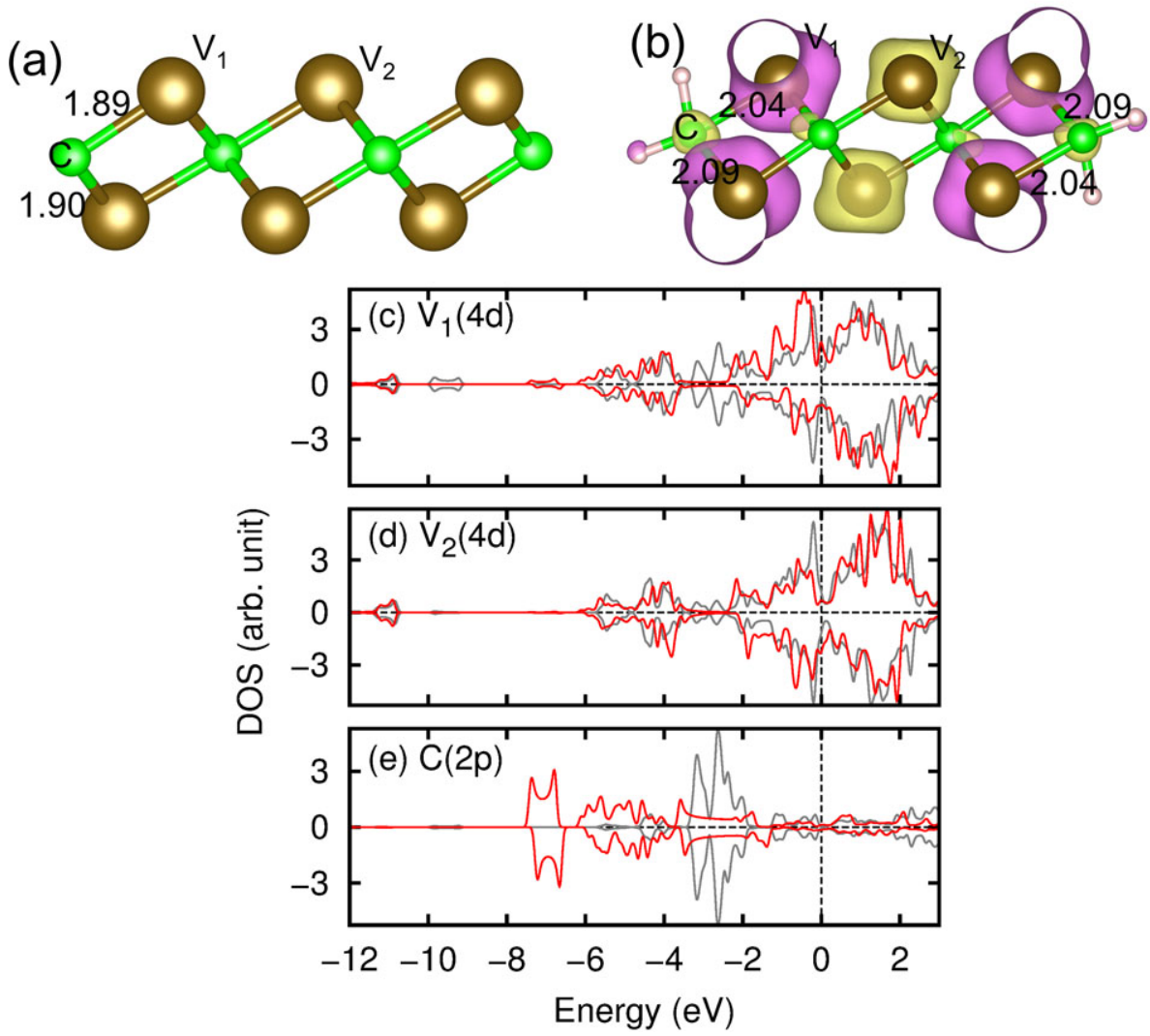

FIG. S10. Spin density plots of bare and hydrogen-passivated 6-CVV-VVC nanoribbons. The isovalue is ± 0.005 e^{-}/au^{3} with positive represented by purple and negative by gold color. Some bonding distances are denoted in angstrom. The PDOS of selected atoms are provided below and the gray and red curves represent the PDOS of atoms in bare and hydrogen-passivated nanoribbons, respectively.