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Manipulation of electrochemical properties of MXene electrodes for supercapacitor applications by chemical and magnetic disorder

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Supporting Information

 Relative formation energies of V_{2-x}Mn_xC, x=0.5, 1.0, 1.5



Fig. S1 The relative formation energies of $V_{2-x}Mn_xC$ for x=0.5, 1.0, 1.5 is shown. The red dashed line indicates the minimum energy configuration for that particular alloying composition and is set at 0 meV/atom. The respective black bars show the range of relative formation energies for the other configurations considered.

In Figure S1, we show the formation energies of the configurations, relative to that of the ground state for each one of the three $V_{2-x}Mn_xC$ compounds. We find that the ground states are lower in energy by about 8 meV/atom at least, thus negating possibilities of near degeneracies in the configurations with respect to the ground state one.

2 Magnetic and chemical environments on the surfaces: correlations with the ground state magnetic properties of $V_{2-x}Mn_xCO_2$

There are 16 transition metal atom positions on either surfaces of $V_{2-x}Mn_xCO_2$ MXene solid solution in the $4 \times 4 \times 1$ supercell used here. The Carbon layer too has 16 positions. On each surface, there are 16 oxygen positions passivating the surfaces. For the ground state of x = 1.5, the atomic arrangements on top and bottom surfaces are shown in Figure S2(a) and (b), respectively. On the top surface, spins of all Mn atoms align along cdirection while on the bottom surface, specific four out of twelve Mn atoms have their spins aligned opposite to c. Each one of these anti-aligned Mn is surrounded by four aligned Mn atoms in a hexagonal environment while each Mn atom, aligned along c, is in the surrounding environment of four Mn atoms, out of which two are also aligned. Two V atoms occupy the remaining vertices of this hexagonal network. In bottom surface the atoms Mn_{13} - Mn_{16} are anti-aligned whereas the rest are aligned. If one considers the hexagon with Mn₁₆, an atom whose spin is aligned opposite to c-direction (the other three with the same spin direction, out of total 12 atoms on this surface, are Mn_{13} - Mn_{15}), at the center, the four Mn atoms Mn₁₉,Mn₂₀,Mn₂₂and Mn₂₄ occupying vertices of the hexagon, have their moments aligned along c. On the other hand, if the hexagon with Mn_{19} at the center is considered, Mn_{21} and Mn_{24} having aligned moments occupy two vertices while Mn₁₅ and Mn₁₆, the two having spins anti-aligned, occupy other two vertices. Such arrangements make the magnetic environment around Mn atoms in the bottom surface inhomogeneous though the chemical environment is homogeneous. Upon inspecting the Mn-Mn bond distances, we find the following: (a) The Mn atoms in the top surface having a moment of 2.7 μ_B are connected to four Mn atoms sitting on the vertices of the

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Fig. S2 Top view of the (a)Top and (b)Bottom surfaces displaying full atomic arrangement in the ground state of $V_{0.5}Mn_{1.5}CO_2$

hexagon around them with Mn-Mn bond distances along a line connecting three Mn atoms (which means two Mn-Mn bonds) between 2.84-2.86 Å and 2.92-2.94 Å For example, consider Mn₄ in Figure S2(a). The Mn₈-Mn₄, Mn₇-Mn₄,Mn₁₀-Mn₄ and Mn₁₂-Mn₄ bond distances are 2.83 Å, 2.93 Å, 2.86 Å and 2.92 Å, respectively. The ones that have their moments slightly reduced have one of the bonds shrunk to 2.75 Å while the other along the same line joining the three Mn elongated to 3.02 Å.For example, Mn₈-Mn₁₀ and Mn₅-Mn₁₀ bond lengths are 2.75 Å and 3.02 Å respectively, while Mn₂-Mn₁₀ and Mn₄-Mn₁₀ distances are more uniform, 2.86 Å and 2.92 Å, respectively. The Mn-V bond distances vary too; for Mn₁-Mn₄, the bond distances are 2.89 Å and 2.93 Å while for the rest 8 Mn, they are 2.84 Å and 3.0 Å rendering the bond lengths along a V-Mn-V line non-uniform, (b) in the bottom surface, when an anti-aligned Mn is connected to four aligned Mn, the two bond distances along a line connecting three Mn atoms are significantly non-uniform, one between 2.68 and 2.72 Å and the other between 3.06 and 3.1 Å For example, in Figure S2(b), Mn₁₆-Mn₂₂, Mn₁₆-Mn₂₄, Mn₁₆-Mn₁₉ and Mn₁₆-Mn₂₀ bond lengths are 3.06 Å, 2.72 Å, 2.68 Å and 3.1 Å, respectively. When an aligned Mn is connected to two anti-aligned atoms, the distribution of bond distances are same. However, the two bond distances for bonds connecting three aligned Mn atoms are 2.77 Å and 3 Å For example, Mn₁₉-Mn₂₄ and Mn₁₉-Mn₂₁ shown in Figure S2(b), similar to the case of Mn in the top layer having a moment of 2.6 µ_B.

The moments on the V atoms on different surfaces can also be correlated to their chemical and magnetic environments. While the V atoms in the bottom surface, located at the center of a hexagon whose vertices have Mn atoms only, have moments of only 0.14 μ_B , the ones in the top layer, sitting in the same environment of Mn, have moments of 0.38 μ_B localised on them. Here



Fig. S3 Top view of the (a)Top and (b)Bottom surfaces displaying full atomic arrangement in the ground state of $V_{1.5} Mn_{0.5} CO_2$



Fig. S4 Top view of the (a)Top and (b)Bottom surfaces displaying full atomic arrangement in the ground state of $V_{1.0} Mn_{1.0} CO_2$

too we find an asymmetry in the Mn-V bond distances in the two surfaces. While the five Mn-V bond distances of the bottom surface vary between 2.87-2.94 Å, one of the Mn-V bonds in the top surface is elongated to 3 Å. Since the spin polarisation in V must be due to the magnetic Mn atoms, a slightly higher moment on V atoms in the top layer can be correlated with the non-uniform Mn-V bond distances.

In Figure S3, the arrangements of atoms on both surfaces of V-rich $V_{1.5}Mn_{0.5}CO_2$ are shown. Each surface has 12 V and 4 Mn atoms. Here each hexagon with a Mn at the center has six V atoms on the vertices. The distribution of Mn-V bond lengths are identical for both surface (There are three Mn-V distances, 3.07 Å, 2.95 Å and 2.72 Å). This can be correlated with identical Mn moments on each atom, irrespective of its location. The V moment is almost zero due to the lack of enough Mn in the neighborhood to polarize V.

In Figure S4, we show the atomic arrangements on the surfaces of $V_{1.0}Mn_{1.0}CO_2$. Here a Mn at the center of a hexagon has four V and two Mn on the vertices while a V at the center of a hexagon has four Mn and two V at the vertices of the hexagon. In this case the bond lengths between the transition metals are again identical for both surfaces. The distribution of bond lengths in the neighborhood of a transition metal atom is also identical with Mn-V bond lengths being 2.82 Å, 2.86 Å, 2.99 Å and 3.02 Å, while Mn-Mn and V-V bonds having identical length of 2.91 Å. Due to no inhomogeneity in magnetic and chemical environment, moments on all Mn atoms are identical. The V is only slightly polarised due to presence of more Mn in its neighborhood in comparison with V-rich compound.

3 Mn and V partial densities of states in ground states of V_{2-x}Mn_xCO₂



Fig. S5 Projected Densities of States of each Mn atom in Ground State of $V_{1.5} \text{Mn}_{0.5} \text{CO}_2$

Mn and V densities of states for $V_{2-x}Mn_xCO_2$ for different *x* in the ground states are shown in Figures S5-S10. The features in the total densities of states shown in the main text can be understood in terms of the features in the atom projected densities of states. We find that the magnetic and chemical environment have significant effect on the atom projected densities of states. The presence of a pseudo-gap in V-rich compound that diminishes as Mn concentration increases, only to re-appear, albeit with



Fig. S6 Projected Densities of States of each V atoms in Ground State of $\mathsf{V}_{1.5}\mathsf{Mn}_{0.5}\mathsf{CO}_2$



Fig. S7 Projected Densities of States of each Mn atom in Ground State of $\mathsf{V}_{1.0}\mathsf{Mn}_{1.0}\mathsf{CO}_2$

strength considerably reduced, for the Mn-rich compound. The sharp pseudo-gap in the electronic structures of V_{1.5}Mn_{0.5}CO₂ is a consequence of strong hybridization of Mn *d*, V *d* and O *p* states. In this compound, the electronic structure of each Mn atom is identical which is a reflection of an identical environment around them, in terms of chemical specie and the bond distances.



Fig. S8 Projected Densities of States of each V atom in Ground State of $\mathsf{V}_{1.0}\mathsf{Mn}_{1.0}\mathsf{CO}_2$



Fig. S9 Projected Densities of States of each Mn atom in Ground State of $V_{0.5} Mn_{1.5} CO_2$

Apart from Mn-V bond distances that are uniformly distributed within the hexagon around an Mn atom, Mn-O, and Mn-C bonds are nearly uniform (Mn-O bond lengths vary between 1.96 Å and 2.05 Å while Mn-C bond lengths vary between 2.03 Å and 2.08 Å). The V partial densities of states, on the other hand, can clearly



Fig. S10 Projected Densities of States of each V atom in Ground State of $V_{0.5} Mn_{1.5} CO_2$

be grouped into two bunches. Eight V atoms (V2, V4, V9, V11, V14, V₁₆, V₂₁ and V₂₃, Figure S5, supplementary material) have identical densities of states with a pseudo-gap like feature around -1 eV in both majority and minority bands. For these V atoms, out of the three V-O bonds, two are significantly smaller (1.76 Å) in comparison to the other (1.88 Å). For the other 16 V atoms, V-O bonds are much longer, between 1.93 and 2.12 Å. Such shorter V-O bonds result in stronger hybridization between d orbitals of V and p orbitals of O leading to the pseudo-gap in the electronic structures. This pseudo-gap like feature is observed in the other 16 atoms at a deeper energy. All Mn and V atoms in the ground state of $V_{1,0}Mn_{1,0}CO_2$ have identical electronic structures. This is expected as the chemical and magnetic environment around each atom is the same. The surfaces have identical spin alignments too. The effect of an increase in Mn content is visible if one compares with the Mn-deficient compound. An increase in chemical disorder smears the main Mn peak observed in the Mndeficient compound, producing a peak and a shoulder. The Mn-V bonds relax as compared to the ones in the Mn-deficient system. In V_{1.5}Mn_{0.5}CO₂, Mn-V bond distances were 2.72 Å and 3.07 Å. In V_{1.0}Mn_{1.0}CO₂, they are 2.82 Å, 2.86 Å, 2.99 Å and 3.02 Å. Such relaxations in the bond lengths reduce the Mn-V hybridizations resulting in the pseudo-gap completely vanishing in the majority spin band and becoming shallow in the minority one. Larger disorder in Mn-rich V_{0.5}Mn_{1.5}CO₂, as compared to the Mn-deficient system now further delocalizes the Mn states (Figure S8, supplementary information). However, sharp peaks and more localization of the majority states is observed for 4 Mn atoms (Mn_1-Mn_4) in the upper surface. For these Mn, the Mn-transition metal bond lengths are more uniformly distributed, varying between 2.83 Å and 2.99 Å. For the other Mn atoms, two Mn bonds along a line joining 3 Mn atoms are severely non-uniform, 2.75 Å and 3.01 Å. The Mn-V bond lengths corresponding to these Mn atoms follow the same trend. Thus, in spite of having identical chemical environments, the larger non-uniformity in bond distances leads to a slightly smaller exchange splitting for these Mn atoms and delocalization in Mn states. The electronic structures of the V atoms are identical as expected. In the bottom surface, the inhomogeneity in the magnetic environments around a transition metal atom affects their electronic structures. Mn_{13} - Mn_{16} have their spins aligned along -c direction and have more localized Mn states as

compared to the other 8 Mn atoms in this surface which have spin orientations opposite to them. They are surrounded by four Mn with spins aligned along c and two V atoms. On the other hand, any one of the other eight atoms on the surface is surrounded by two Mn which have the same spin alignment as the atom in question and two others which have spin alignment opposite to it. This leads to a frustrated triangular network of Mn atoms resulting in a more delocalized electronic structure. The electronic structures of the four V atoms on this surface are identical as they are in identical chemical and magnetic environments. A pseudo-gap-like feature is observed in their minority bands, suggesting slightly stronger hybridization in comparison to that in $V_{1,0}Mn_{1,0}CO_2$. This can be due to slightly shorter and near uniform Mn-V bonds(bond lengths varying between 2.89-2.94 Å). The pseudo-gap-like feature is observed in the top surface Mn minority bands. There too, out of four Mn-V bonds, three vary between 2.84-2.93 Å only.

4 Electronic structure of V_{2-x}Mn_xCO₂ in magnetically disordered states

Total and atom-projected densities of states of $V_{2-x}Mn_xCO_2$ (x=0.5, 1.0, 1.5) for different magnetic disorder (η states) are shown in Figures S11-S13. Section 3 of supporting information discusses the features of the electronic structures of the ground states of each chemical disorder system in detail. In Figure S11(b), we show the densities of states of a PDLM state $\eta = 0.5$ for $V_{1.5}Mn_{0.5}CO_2$. The PDLM state is obtained by flipping the spins of one atom (Mn_4 , Figure S3(a)) from the top surface and three atoms from the bottom surface (Mn_6-Mn_8 , Figure S3(b)). Consequently, the loss of symmetry with respect to the spin orientation affects the electronic structures of different atoms in different ways. That the anti-alignment of spins along *c*-axis has a profound effect on the electronic structure becomes clear from the electronic structure tures for the complete magnetically disordered state $\eta = 0$ (Figure S11(c)). We find that the total densities of states for both spin



Fig. S11 Total, Mn and V Densities of States of V $_{1.5}Mn_{0.5}CO_2$ in (a)Ground (GS), (b) $\eta{=}0.5$ and (c) $\eta{=}0.0$ states.

bands are very similar to that of the ground state. Total and Mn densities of states for $\eta=0.5$ state of $V_{1.0} Mn_{1.0} CO_2$ are shown in Figure S12(c). In comparison with the ground state, We find substantial changes in both spin bands, for energies near Fermi level. The peak in the minority band and the valley, flanked by two peaks, at the Fermi level of the ground state, are absent in this partially disordered state. Densities of states of different Mn atoms undergo noticeable changes from the magnetically ordered ground state. The presence of anti-aligned spins for pairs of Mn forces a change in the exchange field each Mn atom is subjected to, resulting in changes in their electronic structures. When the magnetic disorder is complete ($\eta = 0$), there are further changes in the densities of states close to the Fermi level (Figure S12(c)). In case of $\eta = 0.5$ partial disordered state of V_{0.5}Mn_{1.5}CO₂ too, the electronic structure near Fermi level changes considerably (Figure S13(c)). The pseudo-gap in the minority spin band is now wider in comparison with the ground state. The peak around -1 eV next to the pseudo-gap observed in the ground state has now disappeared. In the complete disordered phase ($\eta = 0$), the electronic structure undergoes further modifications (Figure S13(f)). The changes are prominent in the minority spin band near Fermi level in the occupied part and in both spin bands in the unoccupied part. The densities of states for various partially ordered magnetic states are shown in Figure S12 and Figure S13 for V_{1.0}Mn_{1.0}CO₂ and $V_{0.5}Mn_{1.5}CO_2$, respectively show that there are only slight changes near Fermi level in most cases when η changes. It is also demonstrated that the ordering (or lack of it) of spins and not the number of spins with a particular orientation has a significant impact on the electronic structures. As an example, one can compare the ground state and $\eta = 0.66$ state of V_{0.5}Mn_{1.5}CO₂. The differences in the total densities of states between the ordered ground state and the partially ordered state (Figure S13(a) and (b)) are evident, even though both have the same number of spins aligned along *c*-direction. In a nutshell, the state of magnetic order has non-negligible effects on the electronic structures of $V_{2-x}Mn_xCO_2$ MXenes, particularly for the energies close to the Fermi level.

5 Anomalous charge transfer and its correlation with magnetic environment in $V_{0.5}Mn_{1.5}CO_2$

To understand the unequal charge transfer from the two surface of $V_{0.5}Mn_{1.5}CO_2$ in the ground state, we have shown individual Bader charge on each element before(no-H) and after(with-H) hydrogenation in tables S1(top) and S2(bottom). The results are shown for four non-equivalent atom clusters as marked in Figure S14. Each cluster is denoted by a different colour. From the computed Bader charges, we find that before hydrogenation, all V atoms had an identical charge of 11.07e irrespective of which surface they occupy. After hydrogenation, there is a 0.09e charge more on the V atoms on the top surface. The Mn and C atoms are almost inert in the redox charge transfer through hydrogenation of the surfaces as the changes in the Mn (C) charges after hydrogenation are between 0.04e-0.07e (0.09e-0.12e) only. As expected the surface charge transfer happens through O atoms and the largest changes in charge content happen for them. However, the results suggest that the amount of change depends on the lo-



Fig. S12 Total, Mn and V Densities of States of V_{1.0}Mn_{1.0}CO₂ in (a)Ground (GS), (b) η =0.75, (c) η =0.50, (d) η =0.25 and (e) η =0.00 states.



Fig. S13 Total, Mn and V Densities of States of V $_{0.5}Mn_{1.5}CO_2$ in (a)Ground (GS), (b) $\eta{=}0.66$, (c) $\eta{=}0.50$, (d) $\eta{=}0.33$, (e) $\eta{=}0.16$, and (f) $\eta{=}0.00$ states.

cation of the O atoms. The charge content on the O atoms on the top surface, as a result of hydrogenation, changes between 0.4e-0.52e while for those on the bottom surface, it is between 0.2e-0.34e. The reason behind more charge transfer through the



Fig. S14 Top view of the atomic arrangements in (a)top and (b) bottom surfaces of $V_{0.5} Mn_{1.5} CO_2$. Non-equivalent cluster of atoms are highlighted with different colours.

V atoms could be the rumpling structure of the surfaces in this compound. The rumpling pulls V surfaces closer to the O and thus the H atoms. This is clear from the V-O bond distances that vary between 1.72-1.83 Å whereas the Mn-O bond distances have a wider dispersion (1.92-2.11 Å). The substantially different charge transfer from two surfaces can be correlated with the magnetic environment around an atom on each surface in the ground state of $V_{0.5}Mn_{1.5}CO_2$. Among the O atoms in the bottom surface, O₂₁-O₂₄ (brown block in Figure S14(b)) transfer only 0.17e upon hydrogenation. Each one of these four is networked with an Mn atom which has its spin aligned along -c-direction. The same is true for O_{25} - O_{28} (magenta block in Figure S14(b)) where only 0.19e electrons are transferred. On the other hand, O_{17} -O₂₀ (green block in Figure S14(b)) are networked with 3 Mn out of which 2 have spins aligned along c-direction, the associated charge transfer is 0.33e. A charge transfer of 0.3e happens in case of O₂₉-O₃₂ which are in a network with 2 Mn, both having spins aligned along *c*-direction. Therefore, the presence of at least two Mn having their spins aligned in the same direction enables more charge transfer through the O atoms. All Mn spins on the top surface are aligned in the same direction and the charge transfers associated with O atoms are more. The differences in the amounts of charge transfer for different groups of atoms can be explained through the variations in the transition metal neighborhood of the O atoms. A charge transfer of 0.4e occurs for atoms O_1 - O_4 (orange block in Figure S14(a)). These O have three Mn atoms in their neighborhood. The numbers are 0.4-0.42e for O₅-

O₁₂. Here the O are in a network of two Mn and one V atoms (blue and black blocks in Figure S14(a)) with Mn-O (V-O) bond distances of about 2.0 Å(1.8 Å). The largest charge transfer of 0.52e is associated with the remaining four oxygen (red block in Figure S14(a)) which have the same neighborhood of transition metals as O₅-O₁₂ but the V-O distances are shorter (1.72 Å).

Cluster	Before hydrogenation	After hydrogenation	Atom pair
color code(Figure S14(a))	Atom(charge (e))	Atom(charge (e))	(bond length)
	O ₃ (6.91)	O ₃ (7.31)	-
	Mn ₃ (11.58)	Mn ₃ (11.65)	O_3 -Mn ₃ (1.95)
orange	Mn ₇ (11.60)	Mn ₇ (11.68)	O_3 -Mn ₇ (1.92)
	Mn ₉ (11.60)	Mn ₉ (11.65)	O_3 -Mn ₉ (1.92)
		H ₃ (0.45)	-
blue	O ₇ (6.94)	O ₇ (7.34)	-
	Mn ₄ (11.58)	Mn ₄ (11.65)	O_7 -Mn ₄ (2.00)
	Mn ₇ (11.60)	Mn ₇ (11.68)	O_7 -Mn ₇ (1.99)
	V ₁ (11.07)	V ₁ (11.42)	$O_7 - V_1(1.81)$
	-	H ₇ (0.42)	-
black	O ₉ (6.94)	O ₉ (7.32)	-
	Mn ₁ (11.58)	Mn ₁ (11.65)	O_9 -Mn ₁ (1.98)
	Mn ₉ (11.60)	Mn ₉ (11.65)	O ₉ -Mn ₉ (1.97)
	V ₁ (11.07)	V ₁ (11.42)	$O_9-V_1(1.83)$
	-	H ₉ (0.45)	-
red	O ₁₃ (6.88)	O ₁₃ (7.40)	-
	Mn ₅ (11.60)	Mn ₅ (11.68)	O_{13} -Mn ₅ (2.10)
	Mn ₁₀ (11.60)	Mn ₁₀ (11.65)	O_{13} -Mn ₁₀ (2.04)
	V ₁ (11.07)	V ₁ (11.07)	O_{13} - $V_1(1.72)$
	-	H ₁₃ (0.27)	-

Table S1 Charge on each element on the top surface of $V_{0.5}Mn_{1.5}CO_2$ (Ground state) before and after hydrogenation. Transition metal - oxygen nearest neighbor bond distances (in Å) are also given.

Table S2 Charge on each element on the bottom surface of $V_{0.5}Mn_{1.5}CO_2$ (Ground state) before and after hydrogenation. Transition metal - oxygen nearest neighbor bond distances (in Å) are also given.

Cluster	Before hydrogenation	After hydrogenation	Atom pair
color code(Figure S14(b))	Atom(charge (e))	Atom(charge (e))	(bond length)
green	O ₂₀ (6.91)	O ₂₀ (7.24)	-
	Mn ₁₆ (11.68)	Mn ₁₆ (11.68)	O_{20} -Mn ₁₆ (1.93)
	Mn ₁₉ (11.60)	Mn ₁₉ (11.64)	O_{20} -Mn ₁₉ (1.92)
	Mn ₂₄ (11.58)	Mn ₂₄ (11.64)	O_{20} -Mn ₂₄ (1.92)
	-	H ₂₀ (0.51)	-
brown	O ₂₁ (6.93)	O ₂₁ (7.10)	-
	Mn ₁₃ (11.68)	Mn ₁₃ (11.68)	O_{21} -Mn ₁₃ (2.06)
	Mn ₁₇ (11.60)	Mn ₁₇ (11.64)	O_{21} -Mn ₁₇ (1.99)
	V ₅ (11.07)	V ₁ (11.31)	$O_{21}-V_5(1.78)$
	-	H ₂₁ (0.69)	-
magenta	O ₂₆ (6.91)	O ₂₆ (7.10)	-
	Mn ₁₆ (11.68)	Mn ₁₆ (11.68)	O_{26} -Mn ₁₆ (2.04)
	Mn ₂₂ (11.58)	Mn ₂₂ (11.64)	O_{26} -Mn ₂₂ (1.97)
	V ₅ (11.07)	V ₅ (11.31)	$O_{26}-V_5(1.80)$
	-	H ₂₆ (0.69)	-
violet	O ₂₉ (6.90)	O ₂₉ (7.20)	-
	Mn ₁₉ (11.60)	Mn ₁₉ (11.64)	O_{29} - $Mn_{19}(2.05)$
	Mn ₂₁ (11.58)	Mn ₂₁ (11.64)	O_{29} - $Mn_{21}(2.04)$
	V ₅ (11.07)	V ₅ (11.31)	$O_{29}-V_5(1.75)$
	-	H ₂₉ (0.51)	-