SUPPLEMENTRAY INFORMATION

Metal Dichalcogenide Nanomeshes: Structural, Electronic and Magnetic Properties

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I. PASSIVATED V_{8X}^{4Mo} AND V_{14X}^{6Mo} MOX₂ STRUCTURES

For O passivated V_{8X}^{4Mo} and V_{14X}^{6Mo} MoX₂ monolayers, the unoptimized and optimized passivated V_{8X}^{4Mo} MoX₂ structures are shown in Fig. S1(a,b). The unoptimized passivated V_{8X}^{4Mo} MoX₂ structures are shown in Fig. S1(a). Optimized V_{8X}^{4Mo} MoX₂ (X = S and Se) passivated structures are the same, as shown in Fig. S1(b) and they differed from the unoptimized structure. It is shown that the bond between the 2 Mo atoms in the pore frame is now removed and other bonds are formed. Optimized V_{8Te}^{4Mo} MoTe₂ is similar to them but has more new bonds, as shown in Fig. S1(c). The calculated DOS and PDOS of all passivated V_{8X}^{4Mo} MoX₂ structures are shown in Fig. S1 (d-f) for X = (S, Se and Te), respectively. Fig.



FIG. S1. (a/g) unoptimized passivated $V_{8X}^{4Mo}/V_{14X}^{6Mo}$ MoX₂ (X = S, Se and Te), optimized passivated (b) V_{8X}^{4Mo} MoX₂ (X = S and Se), (c) V_{8Te}^{4Mo} MoTe₂, (h) V_{14X}^{6Mo} MoX₂ (X = S, Se and Te) monolayers, and DOS/PDOS for passivated (d/i) $V_{8S}^{4Mo}/V_{14S}^{6Mo}$, (e/j) $V_{8Se}^{4Mo}/V_{14Se}^{6Mo}$ and (f/k) $V_{8Te}^{4Mo}/V_{14Te}^{6Mo}$. The blue, green, and red balls are the Mo, X, and O atoms, respectively.

S1 (d-f) show that the conduction bands of passivated V_{8X}^{4Mo} MoX₂ structures are dominant

with Mo states and the valence bands of them are dominant with Mo states up to -1.47eV, -1.38 eV and -1.26 eV for X = (S, Se and Te), respectively. The weak contribution of O states appears in the energy range from -0.1 eV to 0.1 eV and from 0.7 eV to 1.1 eVfor X=S, and from 0.6 eV to 1 eV for X=Se, and from 0.57 eV to 0.88 eV for X=Te. The contribution of O states in $\rm V_{8X}^{4Mo}~MoX_2$ is larger than that contribution in $\rm V_{6X}^{1Mo}$ and $\rm V_{6X}^{3Mo}$ due to many X edge atoms in V_{8X}^{4Mo} MoX₂ monolayer. The Fermi level is shifted to the higher energy for X=S and Se structures as compared to the corresponding pristine (Fig. 3) and MoX_2 nanomeshes without passivation (Fig. 7). On the other hand, it shifted to the lower energy for X=Te. New interstitial states are created at the Fermi energy in the gap of the corresponding pristine nanosheets. All passivated nanomesh monolayers are metals which are SC, HM and HM, respectively, before the passivation of the pore. The unoptimized and optimized passivated V_{14X}^{6Mo} MoX₂ structures are shown in Fig. S1(g ,h), respectively. They show that all optimized V_{14X}^{6Mo} MoX₂ passivated structures are the same and they differed from the unoptimized structure since extra bonds are formed. The calculated DOS and PDOS of all passivated V_{14X}^{6Mo} MoX₂ structures are shown in Fig. S1 (i-k) for X = (S, Se and Te), respectively. Fig. 10 (i-k) show that the conduction bands of passivated V_{14X}^{6Mo} MoX₂ structures are dominant with Mo states and the valence bands are dominant with Mo states up to -1.37 eV, -1.27 eV and -1.21 eV for X = (S, Se and Te), respectively. Fermi level shifted to lowe energy for all passivated V_{14X}^{6Mo} nanomesh structures. The contribution of O states in V_{14X}^{6Mo} MoX₂ is larger than that contribution in the previous nanomeshes due to many X edge atoms. The unpassivated V_{14X}^{6Mo} MoX₂ (X= S, Se, and Te) structures are HM, M and HM, respectively, now after being passivated process by O atoms they become metals.

II. PASSIVATED V_{12X}^{7Mo} MOX₂ STRUCTURES

The unoptimized passivated V_{12X}^{7Mo} MoX₂ structures are shown in Fig. S2(a, b), respectively. They show that the all optimized V_{12X}^{7Mo} MoX₂ passivated structures did not differ from the unoptimized structure. The calculated DOS and PDOS of all passivated V_{12X}^{7Mo} MoX₂ structures are shown in Fig. S2 (c-e) for X = (S, Se and Te), respectively. Fig. S2 (c-e) shows that the conduction bands of passivated V_{12X}^{7Mo} MoX₂ structures are dominant with Mo states and the valence bands of are dominant with Mo states up to -1.28 eV, -1.11



FIG. S2. (a) unoptimized and (b) optimized passivated V_{12X}^{7Mo} MoX₂ monolayers, and DOS/PDOS for passivated (c) V_{12S}^{7Mo} , (d) V_{12Se}^{7Mo} and (e) V_{12Te}^{7Mo} . The blue, green, and red balls are the Mo, X, and O atoms, respectively.

eV and 1.35 eV for X = (S, Se and Te), respectively. The contribution of O states in V_{12X}^{7Mo} MoX₂ is approximately similar to that contribution in V_{14X}^{6Mo} due to the same number of X edge atoms.Fermi level shifted to higher energy for V_{12S}^{7Mo} MoS₂ nanomesh structure while it shifted to lower energy for V_{12X}^{7Mo} MoX₂ nanomesh structures where X = Se and Te. V_{12S}^{7Mo} MoS₂ was a half metal before passivation with a gap of 0.2 eV while it is a semiconductor after passivat with a gap of 0.25 eV. On the other hand, new interstitial states are formed around Fermi energy passivated V_{12X}^{7Mo} MoX₂ structures where X = Se and Te converting them to metal structures. Before passivation, they were HM ans SC, respectively.