Supplementary Information

Layered $MoSi_2N_4$ as electrode material of Zn-air battery

Xi-Mei Li, Zheng-Zhe Lin*, Li-Rong Cheng, Xi Chen

1. Clustering of Zn on $MoSi_2N_4$ surface

To compare the processes of Zn intercalating into $MoSi_2N_4$ bulk and clustering on the surface, the add-atom adhesion energy of Zn atom

$$E_{adh}(\mathrm{Zn}) = E(\mathrm{MoSi_2N_4\text{-}Zn}_{n+1}) - E(\mathrm{MoSi_2N_4\text{-}Zn}_{n}) - E(\mathrm{Zn\ atom})$$

is paid attention. Here, $E(MoSi_2N_4 - Zn_n)$ and $E(MoSi_2N_4 - Zn_{n+1})$ are the DFT energies of $MoSi_2N_4$ with n and n+1 Zn atoms, respectively. E(Zn atom)is the DFT energy of an isolated Zn atom. **Figure S1** shows the Zn_n clusters on $MoSi_2N_4$ surface. The Zn adhesion energy E_{adh}(Zn) for the bulk intercalation process along the convex hull (**Figure 2(b)**) and the surface clustering are compared in **Figure S2**. For increasing Zn atom number, E_{adh}(Zn) of bulk intercalation is lower, indicating that bulk intercalation process is more thermodynamically favorable than surface clustering.

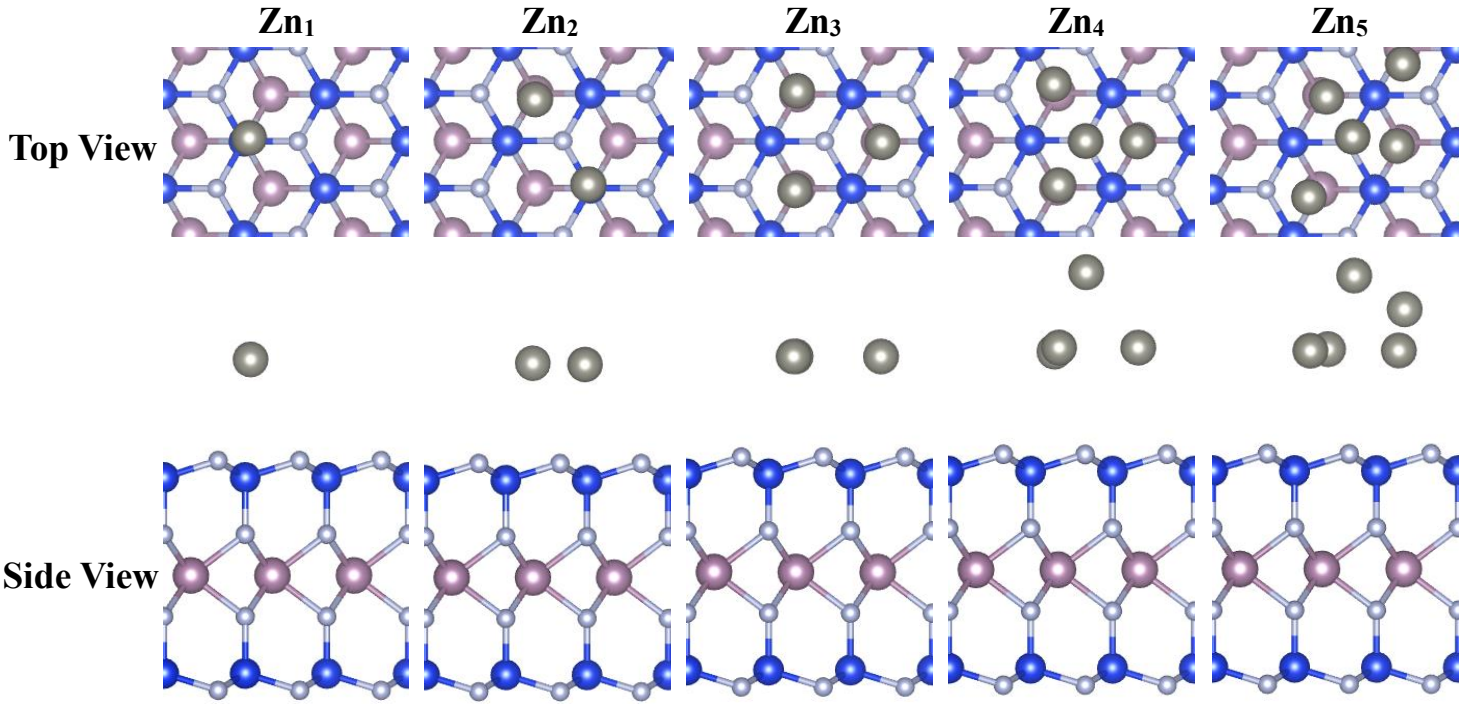

Figure S1 Structures of Zn clusters on $MoSi_2N_4$ surface. Top and side views are shown.

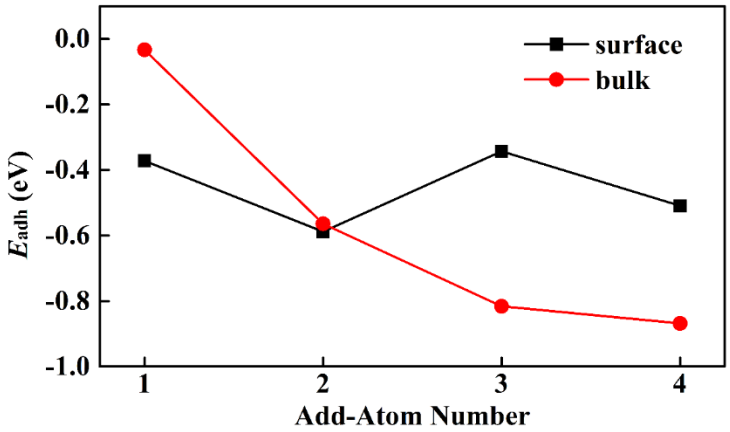

Figure S2 Zn adhesion energy E_{adh}(Zn) for the bulk intercalation process along the convex hull in **Figure 2(b)** and the surface clustering.

2. Adsorption of O_2 on Mxene

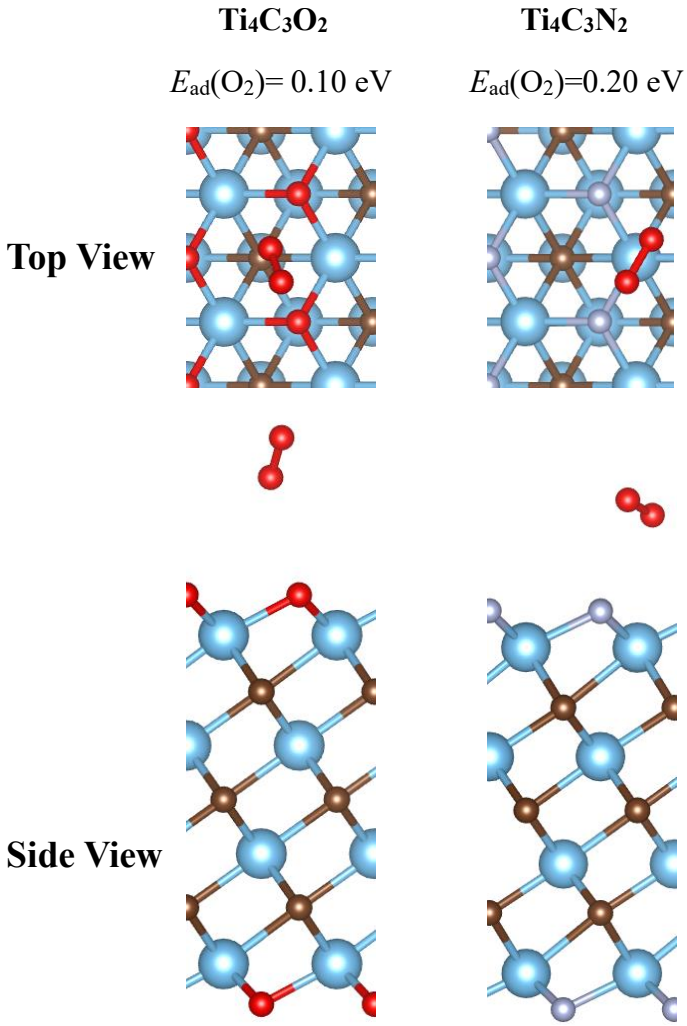

Figure S3 Adsorption of O2 on $Ti_4C_3O_2$ and $Ti_4C_3N_2$. The cyan, brown, red and white atoms are Ti, C, O and N, respectively.

3. The (1-10) lattice plane of $MoSi_2N_4$

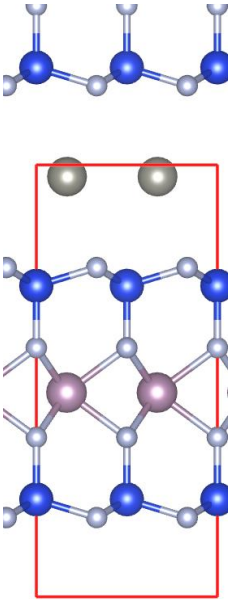

Figure S4 (1-10) lattice plane of $MoSi_2N_4$ shown by the red boundary. The pink, blue, white and gray atoms are Mo, Si, N and Zn, respectively.