

DEVICE APPLICATIONS OF MXENES

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MXenes are members of a new 2D material family of metal carbides and nitrides that could be utilized in nanoscale devices. We have investigated three types of MXene-based nanodevices. First, we have calculated the device characteristics of a magnetic tunnel junction (MTJ). Half-metallic Mn_2CF_2 MXene layer was selected as the magnetic electrode, and structurally compatible Ti_2CO_2 as the transport barrier, as shown in Figure 1. We find that the tunneling magnetoresistance ratio has a peak value of 10^6 . Second, we have considered a $\text{Mo}_2\text{TiC}_2\text{O}_2$ -based quantum transport device as a pressure sensor. In a compressed double MXene, the electronic states originating from the two different transition metals are shifted up unequally. Thus, the character of the valence band maximum (VBM) changes drastically after a critical compression. The proposed nanodevice has moderate pressure sensitivity. While the macroscopic $\text{Mo}_2\text{TiC}_2\text{O}_2$ sensor is usable only for excess pressure detection, the nanodevice can act as a pressure sensor in a wider pressure range. The same mechanism of pressure-induced unequal level-shifting could be exploited also in other double MXenes.

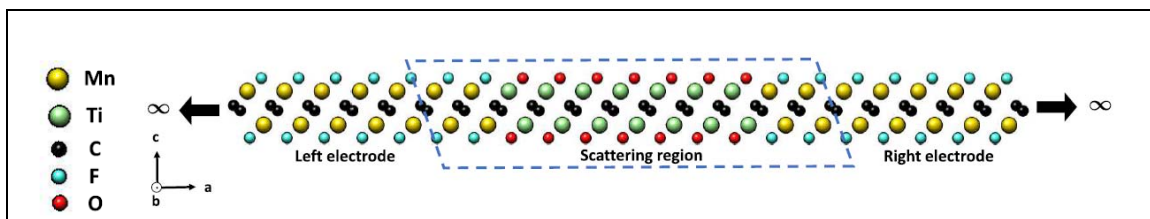


Figure 1. MXene-based MTJ device model.

Third, we propose an MXene-based field-effect transistor, consisting of semiconducting Ti_2CO_2 seamlessly connected to metallic Ti_2CF_2 electrodes of the same family. Our non-equilibrium Green's function (NEGF) quantum transport calculations reveal that the smallest feature size is approximately 6 nm for the gate-controlled current. Changing the surface termination alters the electronic states to allow gate-controlled currents. The positive gate voltages increase the current, while the negative values have the opposite effect. As the surface terminations of the electrodes are not crucial, modification of the termination only in the scattering region is sufficient. The ultrathin Ti_2CT_2 MXene-based nanodevices are thus feasible candidates for efficient field-effect transistors.

Given the excellent stability of MXenes, they are promising ingredients for nanoscale device applications.