Theoretical investigations on the physical properties and fabrication mechanisms of MXenes

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MXene, as a new family of two-dimensional materials, has aroused extensive attentions in recent 6-7 years. Due to their outstanding absorbtion capacities, favorable hydrophilies and conductivities, MXenes were proposed to show widespread potential applications such as in energy storage, sewage disposal and electromagnetic shielding. In this presetation, we systematically studied the structural, mechanical and electronic properties of the carbide MXenes firstly[1]. It implied that the physical properties of the MXenes are significantly depended on the surface functional froups. Moreover, some MXene members show semiconducting characteristics. Based on above, we further investigated the possibility of using those semiconducting MXenes with moderate band gaps (1~2 eV) as the materials for semiconducting devices[2,3]. The key properties of carrier mobility and thermal conductivity were studied. The results shown that the oxygen functionalized M_2CO_2 (M=Ti, Zr, Hf) possess relatively high hole mobilities which are of the order of 10^4 $cm^2V^{-1}s^{-1}$, while Sc_2CT_2 (T=F, OH) MXenes present favorable electron mobilities. The lattice thermal conductivities of these MXenes are significantly related to the metal atom M, where the Sc-containing MXenes generally show higher thermal conductivities than others. With respect to the M_2CO_2 (M=Ti, Zr, Hf) MXenes, their thermal conductivities increase with the increasing atomic number of M, and the room temperature thermal conductivity of Hf_2CO_2 is approximated to that of pure iron. Noteworthily, we have developed a new approach to synthesis MXenes cooperated with experiment. Instead of etching the traditional MAX phases, the layered ternary carbides $M_nAl_3C_{n+2}$ and $M_nAl_4C_{n+3}$ (n equals to 3 or 4) were adopted as precusors, and we have successfully synthesized the Zr- and Hf-containing MXenes [4,5]. The schematic diagram of the synthesis of the $Zr_3C_2T_x$ MXene is shown in Figure 1.

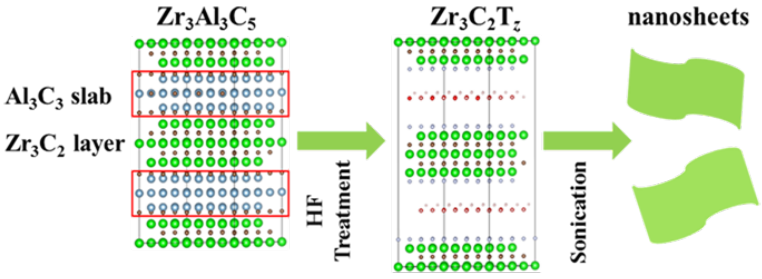

Figure 1. The schematic diagram of the synthesis of $Zr_3C_2T_x$

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