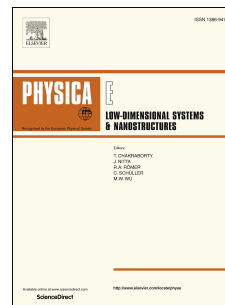


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Structural, Electronic and Mechanical Properties of Two-Dimensional Janus Transition Metal Carbides and Nitrides

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Abstract: Surface functionalization can be used to tune the electronic and mechanical properties of MXenes. In this work, the structural stability, electronic and mechanical properties of monolayer M_2X ($M=Sc, Ti, V, Mn, Nb, Mo, Hf$; $X=C, N$) with asymmetrical functionalization to form Janus MXenes were investigated by first-principles calculations, and the results were compared with the symmetrical functionalization. Results show that asymmetric functionalization has a consequential effect on the structure stability, electronic, elastic properties of the MXenes. For pristine monolayer M_2X ($M=Sc, Ti, V, Mn, Nb, Hf$; $X=C, N$) systems, T-phase is energetically stable than H-phase, whereas the stable structures of monolayers Mo_2C and Mo_2N are H-phase. All the asymmetrically functionalized monolayers M_2X ($M=Sc, Ti, V, Mn, Mo, X=C, N$) except for Sc_2C are metallic materials. A metallic to semiconductor transition occurs in monolayer Sc_2C upon surface functionalization. The mechanical stability of monolayer M_2X can be improved by Janus surface functionalization.

Keywords: Surface functionalization; Monolayer M_2X ; Janus MXenes; Electronic property; Mechanical property; Density functional theory

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