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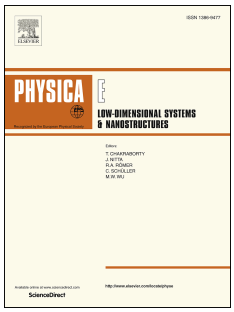


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# Structural, Electronic and Mechanical Properties of Two-Dimensional Janus Transition Metal Carbides and Nitrides

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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