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First-principles investigation of MXenes M4C3 (M = Sc, Cr, and Mn) for clean energy

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The goal of this research is to investigate the structural, optoelectronic, and thermoelectric properties of the MXene, M 4 C 3 (M = Sc, Cr, and M n), using Wien2k code, that is based on density functional theory (DFT). Structural properties and optimization were calculated using PBE-GGA, PBEsol, LDA, and WC approximation. Based on an analysis of the phase stabilities of the carbides, it was found that they are energetically stable, with the following phase stability sequence: Sc 4 C 3 > Cr 4 C 3 > M n 4 C 3 . The band gap 0.784 eV for Sc 4 C 3 is a good gap, compared to the other MXenes. Using the BoltzTraP2 code, the transport properties were thoroughly investigated in terms of electrical conductivity, thermal conductivity, and Seebeck coefficient. The figure of merit (ZT), which is significant for M 4 C 3 , was used to determine its role in clean energy applications.

Primary author: Mr DARKAOUI, El Mokhtar

Presenter: Mr DARKAOUI, El Mokhtar

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