A theoretical study on physical properties of Ti_2InB_2 belonging to a new 212 sub-family of MAX phases

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Abstract: The present study aims to investigate the structural, mechanical, electronic, thermal, dynamic and optical properties of a new and recently synthesized (212) MAX phase Ti_2InB_2compound via the density functional theory (DFT) and to compare with other (211) MAX phases, like Ti_2InC, Ti_2SnC and Ti_2AlC. Our calculated lattice parameters show excellent agreement with the available data. The calculated elastic constants and phonon dispersion spectra confirm mechanical and dynamical stability of the new compound. The studied MAX compounds are found to be brittle in nature. The calculated hardness of the studied MAX compounds shows an excellent agreement with the available experimental and theoretical data with the highest value in the newly synthesized compound Ti_2InB_2.Temperature and pressure dependent thermal properties are investigated through quasi-harmonic Debye model for the first time. The heat capacity of Ti_2InB_2 at room temperature with the inclusion of lattice and electronic contribution is higher than those of other (211) studied MAX phases. The optical reflectivity suggests that the studied MAX compounds are promising candidates as protective coating of other materials against solar heating.