ELECTRONIC STRUCTURES AND THERMAL PROPERTIES OF 312-MAX PHASES

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The "$M_{n+1}AX_n$ phases" (n=1,2, or 3) or "MAX phases", where M is a transition metal, A is an A- group element, and X is either C or N or both, exhibit particular chemical, physical, electrical, and mechanical properties. The unusual properties of the MAX phases can be linked to their layered structures and the nature of bonding. The M-X bonds are strong, while M-A bonds are relatively weak. These mixed metallic-covalent bondings are the source of many exceptional properties of the
MAX phases.

In this work we study a new discovered MAX phase of Zr_3AlC_2, which according to general formula of $M_{n+1}AX_n$, it belongs to the "312" stoichiometry group. We employ Density Functional Theory (DFT)-based methods to obtain electronic structure and lattice dynamics properties. The quasi-harmonic approximation is used to calculate the Helmholtz free energy at temperature range from $10 < T < 1200$ K. For the first time, we predict coefficient of thermal expansion for Zr_3AlC_2 MAX phase. We discuss details and technicalities which are required for accurate calculations of lattice vibration contribution to thermodynamic free energy.