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Structure, bonding and stability of semi-carbides M_2C and sub-carbides M_4C (M=V, Cr, Nb, Mo, Ta, W): A first principles investigation

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Abstract

Density functional theory within the generalized gradient approximation (GGA) is used to investigate the electronic structure and formation energies of semi-carbides M_2C and sub-carbides M_4C (where M=V, Cr, Nb, Mo, Ta and W). Our results show that M_2C carbides are more stable than M_4C. Total and partial densities of states were obtained and analyzed systematically for these phases. Moreover, the bonding nature of M_2C polymorphs is studied from the point of view of the Quantum Theory of Atoms in Molecules (QTAIM). It is found that inter-atomic interactions in these carbides are of mixed type including ionic, covalent and metallic components.

Keywords

- Ab initio calculations;
- Transition metal carbides;
- Phase stability;
- Electronic structure;
- Quantum theory of atoms in molecules