Structure, bonding and stability of semi-carbides M2C and sub-carbides M4C (M=V, Cr, Nb, Mo, Ta, W): A first principles investigation

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Abstract/Résumé : Density functional theory within the generalized gradient approximation (GGA) is used to investigate the electronic structure and formation energies of semi-carbides M2C and sub-carbides M4C (where M=V, Cr, Nb, Mo, Ta and W). Our results show that M2C carbides are more stable than M4C. Total and partial densities of states were obtained and analyzed systematically for these phases. Moreover, the bonding nature of M2C 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/Mots cléfs : Ab initio calculations; Transition metal carbides; Phase stability; Electronic structure; Quantum theory of atoms in molecules

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