STRUCTURAL AND ELECTRONIC PROPERTIES OF AxD1-xByC1-y QUATERNARY ALLOYS VIA FIRST PRINCIPLES

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Abstract

We have investigated the structural and electronic properties of cubic AB, AC, DB and DC compounds and their new AxD1-x ByC1-y quaternary alloys, using the density functional theory. Structural properties of these quaternary alloys are calculated with the Perdew and Wang local-density approximation. The lattice constants of AxD1-x ByC1-y quaternary alloys were computed by Vegards law. The band gap of AxD1-x ByC1-y is related by the compositions x and y. There is no theoretical examining on AxD1-x ByC1-y quaternary alloys and requires experimental confirmation.

Keywords: Structural properties, electronic properties, quaternary alloys

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