Electronic and magnetic properties of $Cr_{3-x}Co_xSi$ alloys - ab-initio study

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Cr_3Si crystallizes in A15-type structure. When Cr_3Si is doped with cobalt, anomalous magnetic properties are observed [1]. Presence of Co leads to appearance of magnetism in Cr_3Si. Total energy calculations for small Co concentrations x=0.0625 and x=0.125 indicate a tendency to clustering of Co atoms [2]. Obtained values of magnetic moments in case of small Co-Co distance are in agreement with experimental reports about ferromagnetism in this alloy, where probably dimerization occurs. The aim of the contribution is to investigate theoretically an influence of Co dopants on electronic and magnetic properties of $Cr_{3-x}Co_xSi$ alloys. Ab-initio calculations will be carried out by the Full Potential – Linearized Augmented Plane Waves with Local Orbitals method implemented in Wien2k code [3] in wide range of Co concentrations.

References:

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