Substitutions' impact on the Curie temperature in Cantor alloy's derivatives

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Multiprincipal element alloys stand for promising materials with a wide range of possible applications *e.g.* in mechanical engineering. One of the most known representatives is the high entropy alloys (HEA). They benefit from composing of several components, which leads to the high-temperature stabilization and variability of their properties. Magnetism and magnetic ordering represent important properties, which the application potential depends on. Not only are they important by themselves, but they influence other properties as mechanical ones. We discuss the enhancement of the magnetism given by nonmagnetic p- and d-substitutions in the well-known Cantor alloy based on the ab-initio calculations. Although the parent alloy is composed of magnetic $3d$ elements, it does not bear noticeable magnetic behavior. Employing the TB-LMTO-ASA method, which allows for an effective including of disorder within the framework of CPA, we describe magnetic exchange interactions in the substituted alloys and determine their magnetic ordering temperatures based on the Monte-Carlo simulations as their knowledge is important for the estimation of their magnetic properties under the ambient conditions. We discuss the difference between the p- and d-typed substitutions and the most suitable composition to achieve ferromagnetic ordering above the room temperature.

References:

[1] J. Šebesta, Karel Carva, and Dominik Legut; Phys. Rev. B 103, 064407 (2021)

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