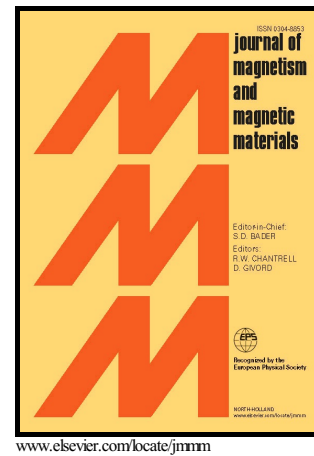


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4-*d* magnetism: electronic structure and magnetism of some Mo-based alloys

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Abstract

We report results of a first-principles density-functional study of alloys of the 4*d*-element Mo with group IV elements Si, Ge and Sn in zinc blende (ZB) and rock salt (RS) structures. The study was motivated by a similar study of ours based on the 4*d*-element Tc, which showed the presence of half-metallic states with integer magnetic moment ($1\mu_B$) per formula unit in TcX (X=C, Si, Ge) alloys. The calculated Curie temperatures for the ferromagnetic (FM) phases were low, around or less than 300 K. Searching for the possibility of 4*d*-based alloys with higher Curie temperatures we have carried out the study involving the elements Mo, Ru and Rh. Among these the most promising case appears to be that involving the element Mo. Among the MoX (X=Si, Ge, Sn) alloys in ZB and RS structures, both MoGe and MoSn in ZB structures are found to possess an integer magnetic moment of $2\mu_B$ per formula unit. ZB MoSn can be classified as a marginal/weak half-metal or a spin gapless semiconductor, while ZB MoGe would be best described as a gapless magnetic semiconductor. The calculated Curie temperatures are in the range 300-700 K. Considering the theoretical uncertainty in the band gaps due not only to the treatment of exchange and correlation effects, but density functional theory itself, these classifications may change somewhat, but both merit investigation from the viewpoint of potential spintronic application. Based on their higher Curie temperatures, Mo-based alloys would serve such purpose better than the previously reported Tc-based ones.

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