Symmetry Induced Half-Metallic Alkaline Earth Ferromagnets

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Search for new half-metallic ferromagnetic binary compounds composed of alkaline earth and III or IV elements (like Boron or Carbon) is reported. Ab initio all-electron density functional theory calculations in the generalised gradient approximation indicate possibility of half-metallic ferromagnetism with Curie temperatures in the range of room temperature. These are a new type of theoretically predicted hypothetical materials without transition metal elements, not yet fabricated. Ferromagnetism is induced by the lack of four-fold crystalline symmetry for lattice constants larger than that of equilibrium for the bulk material. The predominant s-p electron mechanism is responsible for the formation of localised magnetic moments and their interactions.

 $9.7~\mathrm{cm}$

Subject category:

3. Magnetic Structure and Dynamics

Presentation mode:

poster

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