Electronic Band Structure Calculations on Thin Films of the $L2_1$ Full Heusler Alloys X_2YSi (X, Y = Mn, Fe, and Co): toward Spintronic Materials

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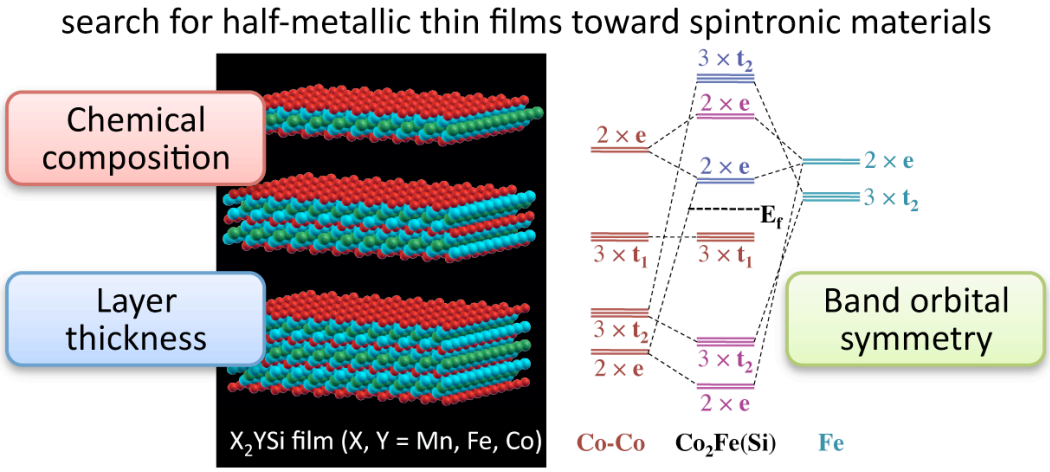
To design half-metallic materials in thin film form for spintronic devices, the electronic structures of full Heusler alloys (Mn_2FeSi, Fe_2MnSi, Fe_2FeSi, Fe_2CoSi, and Co_2FeSi) with an $L2_1$ structure have been investigated using density functional theory calculations with Gaussian-type functions in a periodic boundary condition. Considering the metal composition, layer thickness, and orbital symmetries, a 5-layered Co_2FeSi thin film, whose surface consists of a Si layer, was found to have stable half-metallic nature with a band gap of *ca*. 0.6 eV in the minority spin state. Using the group theory, the difference between electronic structures in bulk and thin film conditions will be discussed.



[1] H. Mori *et al*., *Thin Solid Films*, **520**, 4979–4983 (2012).