Heusler compounds in Spintronics: Theory and Perspectives

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The developments in nanoelectronics, combining the magnetic and semiconducting materials (known as spintronics)[1] or using exclusively magnetic elements (known as magnetoelectronics)[1] have brought the half-metallic magnets,[2] initially predicted by de Groot and collaborators in 1983, to the center of scientific research. In these materials the two spin bands show a completely different behavior. While the spin-up electronic band structure is metallic, in the spin-down band the Fermi level falls within an energy gap as in semiconductors. Such half-metallic compounds exhibit, ideally, a 100% spin polarization at the Fermi level and therefore they should have a fully spin-polarized current and be ideal spin injectors into a semiconductor, thus maximizing the efficiency of spintronic and magnetoelectronic devices.[3]

Heusler compounds are a promising family to achieve half-metallicity since they encompass a large number of members, they crystallize mostly in cubic structures similar to the zincblende structure of semiconductors and several have very high Curie temperatures.[4] Several among them have been predicted to be half-metals and in case of half-metallicity the total spin magnetic moment in the unit cell is intrinsically connected to the total number of valence electrons. This behavior is usually referred to as "Slater-Pauling rules" in literature.[5] Most of them are metals exhibiting diverse magnetic phenomena.

A review on the state-of-the-art of the theoretical description of the half-metallic Heusler compounds will be provided based on first-principles density-functional calculations. Several aspects of their magnetic behavior will be discussed. Particular emphasis will be given to novel functionalities like spin-filtering and magnetic semiconductors. The perspectives of their future use in spintronics devices will be summarized, and preliminary results on novel devices based on Heusler compounds such as superlattices combining half-metallicity of Heusler compounds with perpendicular magnetic anisotropy of binary ferromagnets will be presented.

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