Heusler alloys with physical properties "on request"

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Résumé

Intermetallic systems discovered almost 120 years ago by F. Heusler are an example of an extraordinary variety of physical behaviors of apparently close materials, crystallizing in a simple structure. Heusler alloys include metallic magnets (strong and weak), half-metallic ferromagnets, magnetic semiconductors, semimetals, semiconductors, topological insulators, and even superconductors. The "on request" physical properties occurring in these systems are still a very attractive object of experimental and theoretical research, due to their applications as thermoelectrics, magnetocalorics, shape memory alloys, spintronic materials. Didactically speaking, Heusler systems can serve as an excellent model for studying the usually complex relationships, electron band structure < -> physical properties, taking into account the influence of disorder on phase transitions (e.g. metal-semiconductor, ferromagnet-paramagnet). From this perspective, using the archival and recent electronic structure calculations, I will show the surprisingly fertile concept of the "electronic phase diagram" of half-Heusler alloys proposed in the late 1990s as derived from KKR(CPA) calculations, which helped to understand the diversity of behaviors of these systems, but also to predict new systems with the desired physical properties.

Mots-Clés: electronic structure, Heusler alloys, electron transport, magnetism, KKR, CPA method

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