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Rational Design of Half-Metallic Alloys[1] WILLIAM BUTLER, CLAUDIA MEWES, CHUNSHENG LIU, MINT Center, University of Alabama, MAIRBEK CHSHIEV, Spintec — A half-metal is a material that is a metal for one spin-channel and an insulator or semiconductor in the other. Half-metals are potentially important for spintronic applications such as magnetic sensors for hard drives and magnetic random access memory. We show using very simple ideas that it is possible to rationally design a class of magnetic alloys by placing a gap at the center of one of the d-bands and placing the Fermi energy in this gap. We will present design rules that can be used to make an infinite number of half-metallic heterostructures. We will also show how the half-metallic feature may be maintained at surfaces and interfaces.

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William Butler
University of Alabama

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