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Insight into structural, electronic, magnetic and elastic properties of full-Heusler alloys Co_2YPb (Y = Ti, V, Fe and Mo): A first-principles study

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We have studied the electronic, magnetic and elastic properties of full-Heusler alloys Co_2YPb (Y = Ti, V, Fe and Mo) using FP-LAPW method which is based on DFT implemented in the wien2k code with GGA and modified Becke–Johnson (mBJ) approximations. Electronic and magnetic properties show that Co_2YPb (Y = Ti, V, Fe and Mo) are half-metallic and ferromagnetic. Elastic properties indicate that Co_2YPb are mechanically stable and ductile.

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