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DFT modeling of filled (Fe,Co)P_3 skutterudites for thermoelectricity OLE M. LØVVIK, University of Oslo, KRISTER MANGERSNES, Institute for Energy Technology, Norway, ØYSTEIN PRYTZ, University of Oslo — Skutterudites on the form $M_x Co_{4-y} Fe_y P_{12}$, with Mbeing La, Y, and Sc, x= {0, 0.125, 0.25, 0.50, 1}, and y= {1, 2, 3, 4}, have been studied using band-structure density-functional theory (DFT) calculations. The stability of these hypothetical phases (only two have so far been reported in the literature) has been assessed by comparing to other relevant phases. The Sc-filled compounds, which would have had very large rattling amplitudes due to the small size of the Sc atom, were all shown to be thermodynamically unstable, but several of the La- and Y-filled compounds should be possible to synthesize. The maximum stability was found for the compositions with $y = 3x$. Such compounds also seem to be best suited to thermoelectric purposes from their electronic structure.

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