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First-principles electronic structure of shape-memory alloy Ni_2MnGa[1] BOGDAN MIHAILA, ALICE ACATRINEI, CHRISTOPHER D. TAYLOR, Los Alamos National Laboratory, CYRIL P. OPEIL, Boston College, LLUíS MAÑOSA, Universitat de Barcelona, Catalania — The Ni_2MnGa memory-shape alloy undergoes both a feromagnetic phase trasition ($T_C \sim 380$ K) and a martensitic transformation (MT, $T_M \sim 175$ K) upon cooling. In addition, the MT is preceeded by a premartensitic (pre-MT) phase transition corresponding to a micromodulated structure accompanied by phonon softening presumably related to Fermi-surface nesting and strong electron-phonon coupling. Here, we report results of a comparison study of first-principles electronic structure calculations and recent angle-resolved photoemission measurements, at temperatures T=219 K, in close proximity with the pre-MT, and T=173 K, in the martensite phase.

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