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Electronic Structure Calculations of NiTi Based Ternary Systems[1] HENRY SCHREINER, III, Angelo State University Department of Physics, JUNG-HWAN SONG, NICHOLAS HATCHER, ARTHUR J. FREEMAN, Northwestern University — In this study, the electronic structures of ternary nickel titanium "shape memory" alloys were investigated using a first principles approach within density functional theory. We used the full potential linearized augmented plane wave (FLAPW) method for all calculations, and developed models of the alloys NiTiCu, NiTiFe, and NiTiPd. Both the B2 and the B19' phases for these systems were modeled to determine phase energetics and fundamental mechanisms for structural preference. Splitting of Ni d-states due to Cu and Pd additions and total energy comparisons of the phases explain the effect of ternary additions on changing martensitic transition temperatures. Total energy analysis was used to predict the ground state phase change of NiTiCu B19' to B19 as Cu content increases from 12 at% to 25 at%, which is consistent with recent experiments. Site preferences for Cu and Fe were investigated for same composition alloys. From these results and by predicting alloy properties from first principles, we show how these ab initio calculation methods may be used for designing novel materials.

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