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Magnetic and structural properties of transition metals and their alloys MATTEO COCOCCIONI, KOICHIRO UMEMOTO, University of Minnesota, BURAK HIMMETOGLU, University of California, Santa Barbara — In this talk I will discuss the relationship between magnetic and structural properties emerged from recent DFT calculations on transition-metals and their alloys. In the first part I will present results on Ni_2MnGa, a prototype magnetic Heusler alloy. I will demonstrate that improving the description of localized electrons on the d states of Mn is crucial to fix both the magnetization and the relative stability of the austenite and martensite phases. The larger energy difference between Hubbard bands obtained from DFT+U also proves fundamental to capture the stabilization of the non distorted austenite in alloys with eccess Mn, in agreement with experiments. In the second part I will report our recent discovery of a new phase of bulk Fe. The new allotrope is characterized by a unit cell of six atoms and a crystal structure based on a "wavy" pattern of distorted Fe octahedra. Although always metastable, it is more stable than other known phases (e.g., HCP) and transforms into FCC Fe under pressure. In addition, the distorted crystal structure results in a magnetization density about 10% higher than that of other allotropes which could disclose interesting applications for this materials, including magnetic steels and rare-earth-free permanent magnets.

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