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Effects of the Electronic Doping In the Stability of the Metal Hydride NaH[1] MONICA-ARACELI OLEA-AMEZCUA, JUAN-FRANCISCO RIVAS-SILVA, OMAR DE LA PEÑA-SEAMAN, Institute of Physics (IFUAP), Benemerita Universidad Autonoma de Puebla (BUAP), ROLF HEID, KLAUS-PETER BOHNEN, Institute of Solid State Physics (IFP), Karlsruher Institute of Technology (KIT) — Despite metal hydrides light weight and high hydrogen volumetric densities, the Hydrogen desorption process requires excessively high temperatures due to their high stability. Attempts for improvement the hydrogenation properties have been focus on the introduction of defects, impurities and doping on the metal hydride. We present a systematic study of the electronic doping effects on the stability of a model system, NaH doped with magnesium, forming the alloying system $Na_{1-x}Mg_xH$. We use the density functional theory (DFT) and the self-consistent version of the virtual crystal approximation (VCA) to model the doping of NaH with Mg. The evolution of the ground state structural and electronic properties is analyzed as a function of Mg-content. The full-phonon dispersion, calculated by the linear response theory (LRT) and density functional perturbation theory (DFPT), is analyzed for several Mg-concentrations, paying special attention to the crystal stability and the correlations with the electronic structure. Applying the quasiharmonic approximation (QHA), the free energy from zero-point motion is obtained, and its influence on the properties under study is analyzed.

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