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Stability of alkali-metal hydrides: effects of n-type doping
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Metal hydrides could be considered ideal solid-state hydrogen storage systems, they
have light weight and high hydrogen volumetric densities, but the hydrogen des-
orption process requires excessively high temperatures due to their high stability.
Efforts have been performed to improve their dehydrogenation properties, based
on the introduction of defects, impurities and doping. We present a systematic
study of the n-type (electronic) doping effects on the stability of two alkali-metal
hydrides: Na_{1-x}Mg_xH and Li_{1-x}Be_xH. These systems have been studied within the
framework of density functional perturbation theory, using a mixed-basis pseudopo-
tential method and the self-consistent version of the virtual crystal approximation
to model the doping. The full-phonon dispersions are analyzed for several doping
content, paying special attention to the crystal stability. It is found a doping content
threshold for each system, where they are close to dynamical instabilities, which are
related to charge redistribution in interstitial zones. Applying the quasiharmonic
approximation, the vibrational free energy, the linear thermal expansion and heat
capacities are obtained for both hydrides systems and are analyzed as a function of
the doping content.

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