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Theoretical investigation of catalysed MgH₂ PETER LARSSON, C. MOYSES ARAUJO, Condensed Matter Theory Group, Physics Department, Uppsala University, Box 530, 751 21, Uppsala, Sweden, J. ANDREAS LARSSON, Tyn-dall National Institute, Lee Maltings, Prospect Row, Cork, Ireland, PURU JENA, Department of Physics, Virginia Commonwealth University, Richmond, Virginia 23284-2000, RAJEEV AHUJA, Condensed Matter Theory Group, Physics Department, Uppsala University, Box 530, 751 21, Uppsala, Sweden — MgH₂ has attracted much attention for being a good hydrogen storage material due to its light weight, low manufacturing cost and high storage capacity (7.6 wt%). But its slow absorption/desorption kinetics and high dissociation temperature (nearly 300 °C) limit its practical applications for hydrogen storage. To overcome this, much effort has been paid mainly by making nanocrystalline Mg and/or by adding alloying elements. In this work, we provide a theoretical investigation of the electronic and structural properties of pure and M-doped MgH₂ (with M=Sc, Ti, V, Fe, Ni, Al). We have made calculations for both the crystalline state and 1.0 nm particles. The self-consistent total energy calculations are performed within density functional theory using the VASP package for crystals and TURBOMOLE package for clusters. One aim of this study is to see if the alloying elements can weaken the Mg-H bonds, resulting in improved thermodynamics and faster kinetics. Another one is to understand the differences in the thermodynamics of clusters and crystals.

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