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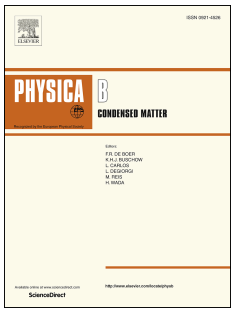

Structural, electronic, dynamic and thermodynamic properties of $Zr_{1-x}Hf_xH_2$ hydride alloys: A first-principles study based on the virtual crystal approximation

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Structural, electronic, dynamic and thermodynamic properties of $Zr_{1-x}Hf_xH_2$ hydride alloys: a first-principles study based on the virtual crystal approximation

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ABSTRACT

The structural, electronic, dynamic and thermodynamic properties of $Zr_{1-x}Hf_xH_2$ (where x is the concentration of constituent element Hf, which changes in the range from 0 to 1 with step size Δx=0.1) are investigated using first-principle calculations. These are done using the density-functional theory (DFT) and density functional perturbation theory (DFPT) within Generalized Gradient Approximation (GGA) and employing virtual-crystal approximation (VCA) method. The lattice constant gradually decreases from 3.527 Å to 3.474 Å with Hf substitute ratio increasing and the variation is quite small. The electronic density of states (DOS) of $Zr_{1-x}Hf_xH_2$ gradually expands when x value varies from 0 to 1 and all of these compounds show metallic nature and the metallicity increases. The analyses of charge density and the charge density differences indicate that the $Zr_{1-x}Hf_x$-H interactions in the hydride are primarily metallic with a small ionic component, and the metallic nature enhances as x increases. Moreover, with Hf substitute ratio increasing, the optical branch and the acoustical branch

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