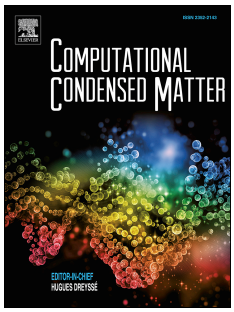
Accepted Manuscript



First principles studies of hydrogen insertion effects on magnetic properties, bonding and structure reordering of UZr_2

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PII: S2352-2143(17)30061-8

DOI: 10.1016/j.cocom.2017.08.001

Reference: COCOM 83

To appear in: *Computational Condensed Matter*

Received Date: 10 April 2017

Revised Date: 20 July 2017

Accepted Date: 3 August 2017

Please cite this article as: S.F. Matar, First principles studies of hydrogen insertion effects on magnetic properties, bonding and structure reordering of UZr_2, *Computational Condensed Matter* (2017), doi: 10.1016/j.cocom.2017.08.001.

First principles studies of hydrogen insertion effects on magnetic properties, bonding and structure reordering of UZr_2.

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Abstract

In the context of the need to recycle depleted uranium coming from nuclear waste, hydrogen absorption in uranium and mainly its alloys is an important solution. We here consider hydrogen insertion in UZr_2 intermetallic leading to experimentally observed composition UZr_2H_6. Drastic changes are shown from density functional calculations to induce atom reordering within the metal substructures in the ground state. Particularly among different starting hypotheses for H sites, energy minimization is observed when the hydrogenated intermetallic undergoes metal substructures reordering with unmixed occupancy of Al (U) and B (Zr) sites in AlB_2 type structure. Hydrogen is identified as covalently bonded within the plane of Zr metal, illustrated by anionic charged $H^{-0.55}$ derived from Bader analysis of charge density. Hydrogen uptake leads to prevailing volume expansion effects versus chemical bonding ones, involving strong localization of uranium 5f states and increased magnetization versus the pristine intermetallic. Both the intermetallic and the ternary hydride are found ferromagnetic in the ground state.

Keywords. *Uranium intermetallics. Hydrides. Magnetism. DFT. AIM. ASW. PAW-GGA*