Electronic properties of $LaNiInH_x$ compounds

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The electronic properties of $LaNiInH_x$ compounds were studied recently [1]. In this work we report the influence of the doped hydrogen on the electronic structure of the $LaNiInH_x$ (x=0, 1/3, 2/3 and 1) compounds which crystallize with ZrNiAl-type structure. The electronic properties were calculated by using ASW method [2].

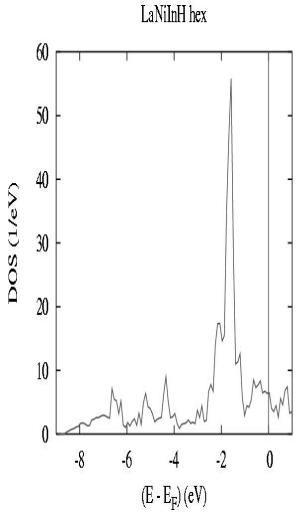

Fig. 1. Total density of states.

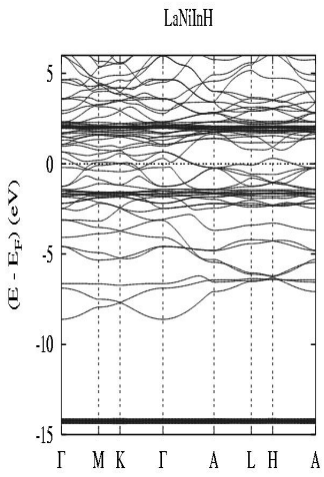

Fig. 2. Band structure.

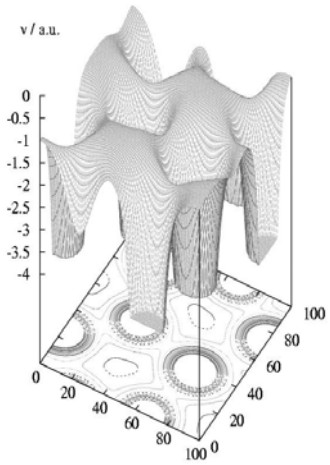

Fig. 3. Charge density.

The hydrogenation does not influence on the crystal structure, however we observe the change of the density of states near the Fermi level, the charge densities and band structure on the position of hydrogen in the unit cell.

[1] A. Jezierski, B. Penc, A. Szytuła, J. Alloys and Compd. **404** (2005) 204
[2] V. Eyert, The Augmented Spherical Wave Method , Lecture Notes in Physics, **719** (2007)

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