Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Structural Stabilities and Electronic Properties of Cobalt Hydrides YASUYUKI MATSUURA, TATSUYA SHISHIDOU, ADSM, Hiroshima University, TAMIO OGUCHI, ISIR, Osaka University, ADSM, Hiroshima University — Cobalt forms ferromagnetic hydrides CoH_x at high pressures of hydrogen [1]. As the hydrogen pressure increases at temperatures 250-350°C, the concentration of hydrogen in the hcp phase monotonically increases, and reaches $x \sim 0.6$ at 7 GPa. At higher pressures, an fcc-based hydride with $x \sim 1.0$ is formed. At ambient pressure and 120 K, hydrogen atoms in the solution with $x \leq 0.26$ are randomly distributed over octahedral interstitial sites [2]. In the solution with $x = 0.34$ ($x \geq 0.38$), hydrogen atoms occupy every third (second) layer. The magnetic moments of the hcp-based hydrides are oriented to the c-axis, and are decreased with increasing hydrogen concentration at a rate of about 0.36 μ_B per hydrogen atom. In this study, we optimize the structural parameters for several structures, and investigate the structural stabilities and related electronic properties by using first-principles calculations. The full-potential linearized augmented plane wave method with the generalized gradient approximation is adopted.

[1] V. E. Antonov, J. Alloys Compd. **330-332**, 110 (2002).
[2] V. K. Fedotov, V. E. Antonov, T. E. Antonova, E. L. Bokhenkov, B. Dorner, G. Grosse, and F. E. Wagner, J. Alloys Compd. **291**, 1 (1999).

Yasuyuki Matsuura
ADSM, Hiroshima University

Date submitted: 14 Dec 2010 Electronic form version 1.4