Ab initio density functional theory (DFT) calculations are performed to study the adsorption of $H_2$ molecules on a Mg(0001) surface. First, the adsorption energy was investigated. In the calculation of the adsorption process of molecular hydrogen, observation showed a physical adsorption of molecular hydrogen rather than chemisorptions. The diffusion process of atomic hydrogen on Mg (0001) was also presented. Finally, we are comparing all of our calculation with results from previous experiments.

**Keyword:** DFT, Adsorption, Diffusion, Mg(0001), $H_2$