Hydrogen Diffusion and Adsorption on WO3 (001) based on First Principles Calculation

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Abstract

Hydrogen reduction of tungsten oxide is currently the most widely applied ultrafine tungsten powder production process. The process has the advantage of short, pollution free and simple production equipment. But it is difficult to effectively control the morphology and particle size of the tungsten powder because of lacking in-depth understanding of the dynamic mechanism of the process. The first-principles calculations are carried out to explore the diffusion and internal adsorption of hydrogen on the WO-terminated surface of WO3 based on the density functional theory. The results show that hydrogen can diffuse from the WO terminal surface to the inside of WO3, the activation energy of diffusion is 46.682 Kcal/mol. It's preferable for hydrogen to diffuse from the surface to the inside than diffuse within the WO3 lattice. The adsorption energy of hydrogen on the WO termination surface of WO3 is 15.093 Kcal/mol, the adsorption energy of hydrogen inside the WO termination surface of WO3 is 14.116 Kcal/mol, which means the hydrogen is easier to adsorb inside the WO3 lattice.

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