Adsorption energy of hydrogen on tungsten (P-10H)

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1. Introduction and theoretical description

In this work we analyse the interaction of (atomic and molecular) hydrogen with tungsten. This material is a firm candidate to form the divertor wall of tokamak-type nuclear fusion reactors, such as the International Thermonuclear Experimental Reactor (ITER) [1]. Since hydrogen has a very sensitive (desired and unwanted) interaction with tungsten, we study its effects and electronic state densities, to analyse the adsorption energy E_{ads} of the system.

In this work, we calculate the adsorption of H and H_2 on tungsten surfaces on the three sites of the cell: top, hollow and bridge. We use a program simulation based on the DFT (density functional theory) implemented in the Open-Source Code Quantum Espresso [2].

The Kohn-Sham equations were solved with the gradient approximation (GGA), using the Perdew-Burke-Ernzerhof (PBE) functional [3], and ultrasoft pseudopotentials of Vanderbilt. Kohn's orbitals were expanded into plane waves and a cut-off value was taken for the energy of 650 eV. We employed a 14 × 14 × 1 k-point grid for integration in the Brillouin zone. Optimization geometry was performed using the Broyden-Fletcher-Goldfarb-Shanno algorithm (BFGS).

Considering E_{ads} as the parameter to be stabilized, we took a slab of 10 atomic layers in the direction (001) with a lattice of 74 atoms. The same size was taken in the perpendicular directions (010), and (100), as shown in Figure 1. In each of these three crystallographic directions of tungsten, we studied different sites and angular dependences. The three characteristic sites that the molecule or atom would find when interacting with the surface are:

Top: the molecule or atom directly interacting with an atom of the surface.

Hollow: the molecule or atom arranged in such a way that it interacts with four surface atoms.

Bridge: The molecule or atom interacting with two atoms on the surface.

We focused to determine the process of adsorption to explain the existence of different impurities in the divertor of the fusion reactor. This development began with the simulation of ion implantation experiments, validated against existing laboratory experimental results [4].

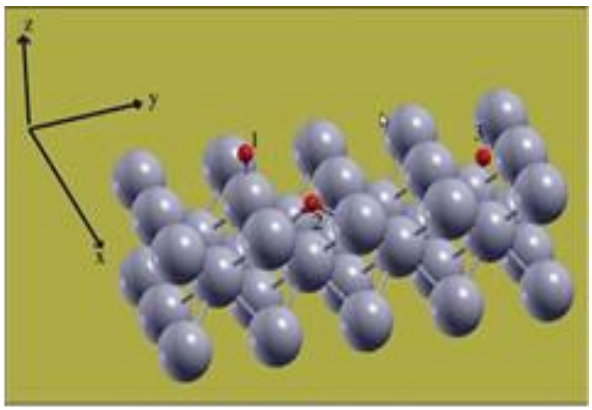

Figure 1: Scheme of the considered system W-atom: (1) top, (2) bridge, (3) hollow interaction sites.

The absorption energy is defined as:

$$E_{ads} = -(E_{molecule/Sup} - E_{Sup} - E_{molecule}), \quad (1)$$

where $E_{molecule/Sup}$ is the energy of the surface-molecule (or atom) system, E_{sup} is the energy of the surface system and $E_{molecule}$ is the energy of the isolated molecule (or atom). Note: The adsorption energy is defined with the opposite sign with respect to the usual definition, for calculation reasons.

2. Results and Conclusions

We analyzed the adsorption energy for atomic H and H_2 molecules. This energy is a surface phenomenon, and each phase (atom or molecule) remains separated.

We obtained a crystallographic network parameter, a=3.162 Å, which diverges from the reference value a= 3.164 Å [6] in less than 0.1%.

Table 1 shows the adsorption energy of the hydrogen atoms. We see that this energy varies appreciably according to the interaction site.

Table 1: Adsorption energy of hydrogen atoms, in eV, in the three different sites of the W crystallographic lattice

Sites	**Top**	**Hollow**	**Bridge**
E_{ads} [eV]	2.96	3.335	3.767

Table 2: Adsorption energy, in eV, of hydrogen molecule in the three different sites of the W crystallographic latticce, for differentes angles of orientation of the molecule, with respect to the W surface.

Site	0°	45°	90°
Top	0.507	0.508	0.009
Hollow	0.006	0.008	0.010
Bridge	0.507	0.514	0.011

From Table 2, it can be seen that the hydrogen molecule is preferentially adsorbed on the Top and Bridge sites, and parallel to the surface (θ= 0°); at θ= 45° the adsorption is almost the same (slightly more favorable for the Bridge site).

For the molecules we found a dependence of the adsorption energy that does not depend much on the chosen crystal orientation, but on the orientation of the molecule. For atoms it is more sensitive.

From our calculation, we must mention that at elevated temperatures there is no significant adsorption probability as hydrogen atoms impinge on the surface.

Finally, we want to highlight the importance of analyzing the adsorption of atomic and molecular hydrogen in tungsten, under the existing conditions in a nuclear fusion reactor such as ITER. In this context, the collisions between hydrogen atoms as well as hydrogen molecules with tungsten surfaces are of great interest, since more than 300 m^2 of the inner surface of the chamber where nuclear fusion will take place is expected to be made of tungsten, as well as the divertor. The studies of probabilities of reflection, absorption, and adsorption of atomic and molecular hydrogen when they strike on a tungsten surface with different crystallographic direction are under way, as well as the findings and challenges of developing a 3-D predictive capability for particle transport in a Tungsten divertor wall.

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