

## DFT Study of Hydrogen in Tungsten: the Role of Monovacancies

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The study of the interaction of Hydrogen (H) isotopes with Tungsten (W) is relevant for the present nuclear fusion research installations such as DEMO and ITER. Tungsten has been proposed as plasma-facing material in these facilities, and will receive deuterium and tritium ions that escape from the magnetic confinement. Experimental measurements on the H-W interaction at relatively low temperature (300-800 K) are difficult because of the low diffusivity and solubility of H in W. Consequently, theoretical studies on H-W interaction are necessary and currently being performed.

In this work ab-initio calculations on the interaction of H with monovacancies in W are performed. For that purpose, density functional theory (DFT) is used.

It is concluded that a monovacancy in Tungsten can retain at least 12 H atoms. Stable configurations of the  $XH_n$  systems ( $X$ =vacancy,  $1 \leq n \leq 12$ ) are proposed.

**Primary author:** BRUZZONI, Pablo (CNEA)

**Presenter:** BRUZZONI, Pablo (CNEA)

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