H Adsorption on Cs/W(110): H-induced Cs Desorption

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Here, we reports results of our study on H adsorption on Cs-decorated W(110) [1], esp., on how the impinging H affects the stability of adsorbed Cs. For reference, we also present the results for H and Cs adsorption on clean W(110). Density functional theory (DFT) based total energy calculation results show decreased adsorption energies for both H and Cs in the presence of the other. H adsorbs more strongly in H/W(110) as compared to the coadsorbed system H/Cs/W(110). We observe the same trend when we compare Cs adsorption in the Cs/W(110) and H/Cs/W(110) systems. Due to the greater electronegativity of H as compared to Cs, increasing the H coverage further weakens Cs adsorption on the W surface. These results suggest that the impinging H could lead to the desorption of Cs from the surface. This explains the observed depletion of Cs and the need for continuous feeding of Cs in fusion applications. This also indicates the need to reevaluate the designs of Cs/W systems used in negative hydrogen production applications. Further details will be discussed at the meeting.

参考文献

[1] *cf., e.g.,* A.A.B. Padama, W.A. Diño, M. Wada, K. Tsumori, M. Kisaki, H. Kasai, H. Nakanishi, M. Sasao, N. Tanaka, *Adsorption of H on Cs/W(110): Impact of H on the Stability of Cs on the Surface*, e-J. Surf. Sci. Nanotechnol. **16** (2018) 391-395.