

# Thermodynamic behavior of the reconstructed W(110) surface induced by hydrogen chemisorption

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We report changes of thermodynamic quantities upon crossing the (1x1) reconstructional phase transition of the W(110) surface induced by hydrogen adsorption. We find that the desorption energy decreases from 40 to 21 kcal/mole while pre-exponential factor drops by six orders of magnitude from 10 to  $10^{-6}$   $\text{cm}^{-1}\text{s}^{-1}$  as hydrogen coverage  $\theta$  changes from 0.5 to 0.75 monolayer(ML). The coverage  $\theta=0.5$  ML matches with the critical coverage where the (1x1) reconstruction begins. We also observe change of total entropy by  $6k_B$  crossing the transition, revealing an active role of substrate reconstruction in reducing the total free energy of the system. Further physical implications of changes of these thermodynamic variables in regard to a driving mechanism of the reconstruction are discussed in detail.

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