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Effect of hydrogen on the surface relaxation of Pd(100) and K/Pd(100)

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Hydrogen induced surface relaxations of Pd(100) and K/Pd(100) have been studied by density functional theory calculations. We find that the first interlayer spacing of Pd(100) expands almost linearly with hydrogen coverage. This result is used to estimate the amount of remaining hydrogen atoms on the surface samples investigated in previous low-energy electron diffraction (LEED) studies, unusually large top-layer expansions of which have been suggested due to hydrogen contamination [1]. The estimated H coverages of 0.6 ~ 1.0 ML, unexpectedly high for the samples claimed as clean, indicates that Pd(100) is extremely susceptible to H contamination, requiring a more careful surface cleaning process. Evidence of H contamination is also found in the K adsorbed Pd(100) surface. Our calculations predict that the K/Pd(100)-c(2x2) surface undergo a rumpling of the second Pd layer of ~0.05 Å at hydrogen coverage of 0.25 ML, while the rumpling vanishes without hydrogen. This result strongly suggests a hydrogen contamination of the K adsorbed Pd(100)-c(2x2) sample investigated in a previous LEED study [2], the second Pd layer of which is rumpled with a splitting of 0.04 Å.

[참고문헌]

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