Subsurface bonding of hydrogen in transition metals: dependence on surface orientation

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The calculation of the surface-induced enhancement of the binding energy of hydrogen impurities in transition metals, previously reported for close-packed surfaces, are extended to open surfaces in the fcc and bcc structures. The effect is found to be stronger for close-packed surfaces than for open ones. Numerical values for the subsurface bonding energy in Nb and Pd are given, from which changes in the kinetics of hydrogen absorption through specific surfaces are predicted.