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Surface states localization induced by single adatoms at metal surfaces SIMONA ACHILLI, Dept. Material Science, University of Milan Bicocca, MARIO ITALO TRIONI, CNR – National Research Council of Italy, ISTM — The perturbation introduced at metal surfaces by the adsorption of a single adatom affects the surface states. Due to their two dimensional character, localized bound states could result at energy lower than the pristine surface states. The extent of such a localization depends on a variety of aspects such as the attractive strength of the adatom induced potential, the adsorption distance, the nature of the surface state. We investigate this effect through a density functional theory approach that accounts for the semi-infinite character of the substrate and which reproduces the experimental surface states and the surface projected energy gap. The results obtained for different kind of adatoms (both magnetic and paramagnetic) on metal surfaces are discussed, focusing on the localization of the Shockley state and of the image states for different adsorption configurations. The spin splitting of the localized bound state will be also analyzed for magnetic adatoms.

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