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Surface magnetism of Fe/W(110): an ab-initio study of the substrate effects TORSTEN ANDERSEN, WOLFGANG HÜBNER, Dept. of Physics, Kaiserslautern University, Box 3049, D-67653 Kaiserslautern, Germany — The pseudomorphic monolayer of Fe grown on a W(110) surface is very interesting from the point of view of magnetism. In studies of the surface magneto-crystalline anisotropy, the Fe monolayer on top of a W substrate has become the system of choice, since (a) the growth of the first Fe monolayer is pseudomorphic, (b) the W substrate has a large spin-orbit coupling, and (c) the interface anisotropy is the strongest ever observed. This makes the Fe monolayer on a W substrate a good candidate for an *ab initio* benchmark investigation of how the properties of the magneto-crystalline anisotropy are influenced by the substrate. Our investigation is done as a function of the substrate thickness (up to 8 layers). Analyzing the magnetocrystalline anisotropy energies, we find stable (with respect to the number of substrate layers) in-plane easy and hard axes of magnetization along the $[1\bar{1}0]$ - and $[001]$ -directions, respectively, reaching a value in good agreement with experiment for thick substrates. Additionally, the magnetic spin- and orbital moments, and the density of the Fe *d*-states are analyzed at different numbers of substrate layers as well as with respect to the direction of magnetization, confirming recent observations that “Hund’s 3rd rule is broken” for the W substrate.

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