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Electronic Structure of Epitaxial Single-Layer MoS_2 PHILIP HOFMANN, JILL MIWA, SøREN ULSTRUP, SIGNE G. SøRENSEN, MACIEJ DENDZIK, ANTONIJA GRUBIŠIĆ ČABO, MARCO BIANCHI, JEPPE VANG LAURITSEN, Department of Physics and Astronomy, Aarhus University — The electronic structure of epitaxial single-layer MoS_2 on Au(111) is investigated by angle-resolved photoemission spectroscopy. Pristine and potassium-doped layers are studied in order to gain access to the conduction band. The potassium-doped layer is found to have a (1.39±0.05) eV direct band gap at $\bar{K}$ with the valence band top at $\bar{\Gamma}$ having a significantly higher binding energy than at $\bar{K}$. The moiré superstructure of the epitaxial system does not lead to the presence of observable replica bands or minigaps. The degeneracy of the upper valence band at $\bar{K}$ is found to be lifted by the spin-orbit interaction, leading to a splitting of (145±4) meV. This splitting is anisotropic and in excellent agreement with recent calculations. Finally, it is shown that the strength of the potassium doping is k-dependent, leading to the possibility of band structure engineering in single-layers of transition metal dichalcogenides.

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