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Semiconductor to Metal Transition in WS2/Ag(111) CHARLOTTE SANDERS, MACIEJ DENDZIK, ALBERT BRUIX, Aarhus University, MATTEO MICHIARDI, University of British Columbia, ARLETTE NGANKEU, MARCO BIANCHI, BJRK HAMMER, JILL MIWA, PHILIP HOFMANN, Aarhus University — Substrate effects play an important role in determining electronic structure in two-dimensional materials (2DMATs). A common effect of a metallic substrate on a semiconducting 2DMAT is strong renormalization of the band gap, induced by metallic screening, as recently observed in MoS2/Au(111) [1]. Here we report a substrate effect that goes beyond a band gap change due to screening. For WS2/Ag(111), interaction with the substrate leads to a pronounced change of the band structure of WS2, from a direct band gap semiconductor to a metal. In this transition, the local minimum in the conduction band at the Q point is pulled down in energy relative to the absolute minimum at K. The Q band minimum can even become lower than the K minimum and cross the Fermi level, becoming partially occupied. This is evident in measurements by angle-resolved photoemission spectroscopy (ARPES); the metallicity of WS2 is also indicated by a characteristic asymmetric lineshape observed in core-level photoemission spectra. ARPES and time-resolved ARPES measurements confirm that the conduction band at K remains above the Fermi level. Reasons for this band distortion are investigated, with reference to band structure calculations based on density functional theory. [1] Phys. Rev. B 93, 165422 (2016)

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