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Direct observation of the indirect to direct band gap transition in epitaxial monolayer $MoSe_2$ film YI ZHANG, LBNL, TAY-RONG CHANG, National Tsing Hua Univ., BO ZHOU, LBNL, YONG-TAO CUI, HAO YAN, ZHONGKAI LIU, FELIX SCHMITT, JAMES LEE, ROB MOORE, Stanford Univ., YULIN CHEN, Univ. of Oxford, HSIN LIN, Northeastern Univ., HONG-TAY JENG, National Tsing Hua Univ., SUNG-KWAN MO, ZAHID HUSSAIN, LBNL, ARUN BANSIL, Northeastern Univ., ZHI-XUN SHEN, Stanford Univ. — As a class of graphene-like two-dimensional materials, the layered metal dichalcogenides MX_2 (M = Mo, W; X = S, Se, Te) have gained significant interest due to the indirect to direct band gap transition in monolayer. Because of this direct band gap, monolayer MX_2 is favorable for optoelectronic applications. Here we report the direct observation such band gap transition by using angle-resolved photoemission spectroscopy on high-quality thin films of $MoSe_2$, with variable thickness from monolayer to 8 monolayer, grown by molecular beam epitaxy. The experimental band structure indicates a stronger tendency of monolayer $MoSe_2$ towards direct band gap, and with larger gap size, than theoretical prediction. Moreover, we observed a significant band splitting of ~ 180 meV at valence band maximum of a monolayer $MoSe_2$, which was theoretically predicted to be 100% spin-polarized. This spin signature gives the layered $MoSe_2$ great application potential in spintronic devices, as well as a new playground to investigate spin-obit physics beyond the topological insulators.

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