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Study of the Valley Hall effect in hydrogen-doped MoS2 by DFT simulation GI WAN JEON, KUE WON LEE, YEOJIN LEE, CHEOL EUI LEE[1], Department of physics, Korea Univ — Molybdenum disulfide (MoS2) is one of the most interesting 2D honeycomb structure transition-metal dichalcogenide (TMDC). MoS2 has intrinsic valley physics and show the valley Hall effect induced by circular-polarized light. In this work, we study hydrogen-doped MoS2 single layer to understand various changes due to hydrogen doping. By controlling the hydrogen position in MoS2 layer and change hydrogen concentration by increase the super cell size, we investigated the valley Hall conductance, band structure, spin density and PDOS.

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