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Electron-doping by hydrogen in transition-metal dichalcogenides
SEHOON OH, SEONGIL IM, HYOUNG JOON CHOI, Department of Physics and IPAP, and Center for Computational Studies of Advanced Electronic Material Properties, Yonsei University, Seoul 03722, Korea — Using first-principles calculations, we investigate the atomic and electronic structures of 2H-phase transition-metal dichalcogenides (TMDC), 2H-MX_2, with and without defects, where M is Mo or W and X is S, Se or Te. We find that doping of atomic hydrogen on 2H-MX_2 induces electron doping in the conduction band. To understand the mechanism of this electron doping, we analyze the electronic structures with and without impurities. We also calculate the diffusion energy barrier to discuss the spatial stability of the doping. Based on these results, we suggest a possible way to fabricate elaborately-patterned circuits by modulating the carrier type of 2H-$MoTe_2$. We also discuss possible applications of this doping in designing nano-devices. This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2016-C3-0052).

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