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Wavefunction Properties and Electronic Band Structures of High-Mobility Semiconductor Nanosheet MoS_2 SEUNG SU BAIK, 1. Center for Computational Studies of Advanced Electronic Material Properties and 2. Dept. of Physics and IPAP, Yonsei University, Korea, HEE SUNG LEE, SEONGIL IM, Dept. of Physics and IPAP, Yonsei University, Korea, HYOUNG JOON CHOI, 1. Center for Computational Studies of Advanced Electronic Material Properties and 2. Dept. of Physics and IPAP, Yonsei University, Korea, CCSAEMP TEAM[1], EDL TEAM[2] — Molybdenum disulfide (MoS_2) nanosheet is regarded as one of the most promising alternatives to the current semiconductors due to its significant band-gap and electron-mobility enhancement upon exfoliating. To elucidate such thickness-dependent properties, we have studied the electronic band structures of bulk and monolayer MoS_2 by using the first-principles density-functional method as implemented in the SIESTA code. Based on the wavefunction analyses at the conduction band minimum (CBM) points, we have investigated possible origins of mobility difference between bulk and monolayer MoS_2. We provide formation energies of substitutional impurities at the Mo and S sites, and discuss feasible electron sources which may induce a significant difference in the carrier lifetime. This work was supported by NRF of Korea (Grant Nos. 2009-0079462 and 2011-0018306), Nano-Material Technology Development Program (2012M3a7B4034985), and KISTI supercomputing center (Project No. KSC-2013-C3-008).

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