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Effect of hydrogen adsorption on the structure of the basal plane of MoS_2[1] DUY LE, ZAHRA HOOSHMAND, TALAT S. RAHMAN, Department of Physics, University of Central Florida — The ability to generate and tailor sulfur vacancies on the basal plane of transition metal dichalcogenide is of interest because it opens the way to utilize the material for catalytic applications. We will present our density functional theory based study of the effect of H_2 adsorption on the structure of the basal plane of single-layer MoS_2. We will show that the 1T phase of MoS_2 can be a catalyst for H_2 dissociation, that the dissociation barrier is about 1.15 eV, and that the resultant atomic H can extract S atoms from the basal plane to create vacancies after overcoming a barrier of 0.15 eV. In contrast, H_2 is found to have hardly any effect on the 2H phase of MoS_2. Moreover, in the lateral heterostructure composed of the 2H and 1T phases of single-layer MoS_2, the spillover of atomic hydrogen from the 1T to 2H phase is expected. Once the atomic hydrogen is on the 2H phase, it is mobile and also has the propensity to bind with sulfur atom to form vacancies. We will also discuss the effect of temperature and pressure on defect creation on the basal plane of MoS_2.

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