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Three, Two and One-dimensional MoS2: A First Principle Investigation CAN ATACA, ETHEM AKTURK, SALIM CIRACI — This study presents our study on atomic, electronic, magnetic and phonon properties of three, two and one dimensional honeycomb structures of molybdenum disulfide (MoS_2) using first-principles pseudopotential plane wave method. The dimensionality effects on various properties are examined. The calculations of phonon frequencies indicate the stability of two dimensional, single layer MoS_2, which consists of a positively charged molybdenum atomic plane between two negatively charged sulfur atomic planes. Three and two dimensional MoS_2 are semiconductors. Their band gaps are calculated within density functional theory and corrected by GW_0 self energy method. Specific foreign adatoms can be chemisorbed at the sulfur plane of the single layer of MoS_2 with significant binding energy and attribute magnetic properties. While bare MoS_2 armchair nanoribbons are nonmagnetic semiconductors, zigzag MoS_2 nanoribbons are ferromagnetic metals. Vacancy defects in bare armchair and bare zigzag nanoribbons affect also the magnetic state and electronic structure of nanoribbons. Variation of the total energy and atomic structure with stretching of nanoribbons exhibit sequential elastic and yielding stages. In the harmonic elastic deformation range force constant and in-plane stiffness are calculated. Plastic deformation with irreversible structural transformation can lead to dramatic changes in honeycomb structure.

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