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Excitonic properties of hydrogenated single-layer MoS_2[1] NASEEM UD DIN, VOLODYMYR TURKOWSKI, TALAT RAHMAN, University of Central Florida — The excitation spectrum of hydrogenated single-layer MoS_2 are investigated systematically using the first-principle Density-Matrix Time-Dependent Density-Functional Theory, for varying hydrogen coverage. In particular, it is shown that the fully-hydrogenated system is metallic, while in the low-coverage limit the spectrum of single-layer MoS_2 acquires spin-polarized partially filled mid-gap states. These states are defined by the orbitals of H atoms which make a tilted bond with the surface S atoms. Our calculated absorption spectrum of the system reveals several excitonic peaks, including states that involve the mid-gap levels. Detailed analysis of the properties of these excitons shows that, similar to the case of pristine single-layer MoS_2, binding energies of the excitons of the hydrogenated system are large (few tenths of an eV), making their experimental detection facile and suggesting hydrogenation as a knob for tune the optical properties of single-layer MoS_2. Comparisons are made with on-going experimental observations. To gain further insights, we examine the effect of alkali coverage (Li and Na) on the optical properties of single-layer MoS_2 and compare them with those of the hydrogenated system.

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