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A first-principles study of the role of defects and electron correlations in monolayer molybdenum disulfide[1] CHINEDU EKUMA, DANIEL GUNLYCKE, U.S. Naval Research Lab — Low-dimensional materials, including monolayer MoS_2, are increasingly being explored for 21st-century device applications. These materials often contain intrinsic defects, which present both opportunities and challenges. To take advantage of such defects, we need a better understanding of the interplay between defects and electron interactions, which are significant in low-dimensional materials. Using our first-principles-based approach for electron localization, we have calculated the typical local density of states and charge susceptibility at various sulfur vacancy concentrations and electron-electron interaction strengths. The local density of states suggest the existence of a correlation-assisted insulator-metal transition. From the charge susceptibility, we have predicted the optical adsorption spectra in the presence of defects and electron interactions. These spectra show exciton peaks in good agreement with experiment.

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