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Thickness dependence of Electron Energy Loss Spectra (EELS) of MoS2 films[1] FENG XUE, State Key Laboratory of Surface Physics, Key Laboratory of Computational Physical Sciences, and Department of Physics, Fudan University, Shanghai , XINXU YAN, Department of Materials Science and Chemical Engineering, University of California, Irvine, ZHE WANG, State Key Laboratory of Surface Physics, Key Laboratory of Computational Physical Sciences, and Department of Physics, Fudan University, Shanghai , HUI WANG, XIAOQING PAN, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine — Band structures and optical properties of monolayer, bilayer, and bulk MoS2 are studied using the GW approximation in conjunction with the Bethe-Salpeter equation (BSE). The calculated electron energy loss spectra (EELS) of these systems show peak structures that depend on the thickness. In particular, the pronounced peak near 3 eV moves to lower energy with the increasing of film thickness. Through analysis of transition matrices and density of states, we attribute this peak shift to modifications of the band structures through the weak interlayer van der Waals interaction. Comparison between theory and experiment are made to reveal the physical insights and to provide guidance for the utilization of novel two-dimensional materials.

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