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The Electronic and Optical Properties of Manganese-doped Wurtzite ZnO YIMING MI, XINXIN ZHAO, School of Fundamental Studies, Shanghai University of Engineering Science, SHUICHI IWATA, Graduate School of Frontier Sciences, The University of Tokyo — The electronic and optical properties of Manganese-doped Wurtzite ZnO were studied by the first principles pseudopotential plane wave method within density functional theory formalism. The electronic structures, density of states, and optical absorption spectra were investigated for different doping concentration. The acquired results reveal that the energy gap of the Mn-doped ZnO increases with the increase of Mn-doping concentration, and the UV absorption of the system gets stronger with the Mn-doping concentration augmented, which are consistent with others' calculational and experimental results fairly well.

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