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Effects of Paramagnetism and Electron Correlations on the Electronic Structure of MnO: *Ab Initio* Study SANGMOON YOON, KYOUNG-SUK JIN, Seoul Natl Univ, SEOUNG-HUN KANG, Kyung Hee Univ, KI TAE NAM, MIYOUNG KIM, Seoul Natl Univ, YOUNG-KYUN KWON, Kyung Hee Univ — Manganese oxide nanoparticles have attracted a lot of attentions as a promising candidate for next-generation catalyst. Therefore, understanding the electronic structure of manganese oxide in room temperature is highly required for the rational design of catalysts. We study the effects of paramagnetism and electron correlations on the electronic structure of MnO using *ab initio* density functional theory. Spin configurations of paramagnetism are postulated as the ensemble average of various spin disorders. Each initial disordered spin configuration is randomly generated with two constraints on magnetic local moments. We first investigate the influence of magnetic ordering on the elctronic structure of MnO using noncollinear spin calculations and find that the magnetic disorders make valence band maximum more delocalized. Moreover, we examine the role of electron correlations in the electronic structure of paramagnetic MnO using DFT+U calculations. Strong electron correlations modify not only the size of band gap but also the magnitude of local moments as in the antiferromagnetic MnO. Besides, the initialized spin disorder remains almost unchanged as electron correlation get stronger. Furthermore, our results obtained by considering both strong electron correlation and paramagnetism confirm experimentally-observed oxygen K edge X-ray emission spectra [1] reflecting the feature of valence bands. [1] E. Z. Kurmaev et al., Phys. Rev. B. **77**, 165127 (2008).

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