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Density functional study on d-orbital characters of the Fe magnetic moment in BaFe₂As₂ HYUNGJU OH, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University — There have been many published papers related on the orbital characters of band structures in the iron-based superconductors. However, the orbital characters of the Fe magnetic moment still remain unrevealed. By performing first-principles calculations of the electronic and magnetic properties with constraint on the real space shape of Fe magnetic moments, we study the d-orbital characters of the Fe magnetic moment in BaFe₂As₂. We compare obtained band structures with published angle-resolved photoemission spectroscopy (ARPES) result, and propose that the Fe magnetic moment in BaFe₂As₂ has in-plane d_{xy} character. This work was supported by the NRF of Korea (Grant Nos. 2009-0081204 and 2011-0018306). Computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2011-C3-05)

Hyungju Oh
Department of Physics and IPAP, Yonsei University

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