

YBaCo₂O₅ 화합물에서의 구조변형에 의한 전하, 궤도, 스핀상태 전이 연구

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Charge and Orbital Ordering and Spin State Transition Driven by
Structural Distortion in YBaCo₂O₅

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초록

We have investigated electronic structures of antiferromagnetic YBaCo₂O₅ using the local spin-density approximation (LSDA) + U method. The charge and orbital ordered insulating ground state is correctly obtained with the strong on-site Coulomb interaction. Co^{2+} and Co^{3+} ions are found to be in the high spin (HS) and intermediate spin (IS) state, respectively. The tetragonal to orthorhombic structural transition is responsible for the ordering phenomena and the spin states of Co ions. The large contribution of the orbital moment to the total magnetic moment indicates that the effect of the spin-orbit coupling is very important in YBaCo₂O₅.

참고 문헌

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