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Electronic properties investigation of YBaCuO using the PAW formalism SIMON PESANT, MICHEL CÔTÉ, Département de physique and Regroupement québécois sur les matériaux de pointe (RQMP), Université de Montréal, Canada — Using density-functional theory (DFT) and the projector-augmented wave (PAW), we characterize the electronic properties of the $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$. These systems are metallic or antiferromagnet at room temperature depending on the hole doping induced by oxygen atoms in the basal plane. Also, the impact of an onsite coulomb repulsion term on the DFT known as LDA+U, is investigated in the different structures to take into account the highly correlated character of the electrons of those systems. The addition of an onsite coulomb repulsive term does not strongly alter the electronic properties of the $\text{YBa}_2\text{Cu}_3\text{O}_7$, and $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$ but gives more accurate details about the electronic structure. In the case of $\text{YBa}_2\text{Cu}_3\text{O}_6$, the impact of the U term is primordial, the anti-ferromagnetism phase being recovered when LDA+U is used, compared to the standard LDA where it is metallic.

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