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Surface effects in Co-doped ZnO nanocrystals[1] ALINE L. SCHOENHALZ, GUSTAVO M. DALPIAN, Universidade Federal do ABC — Semiconducting nanostructures have received high attention by scientific community due to their unusual properties and wide rage of possible applications. In this scale, the understanding of the surface effects of the material is fundamental to explain its properties. By using the Density Functional Theory within the Local Density Approximation, we report on the effects of the surface on the magnetic properties of Co-doped ZnO nanocrystals. For bulk ZnO, it is well known that the most stable magnetic interaction between Co impurities is antiferromagnetic. This is also the case for saturated nanostructures, where surface effects are not taken into account. However, when surface effects are considered, the interaction between transition metal impurities becomes ferromagnetic. We will discuss the interaction between surface and impurity states, comparing our results to experimental findings.

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