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Ferromagnetism driven by extended defects in nanostructured ZnO¹ ALINE L. SCHOENHALZ, JEVERSON T. ARANTES, ADALBERTO FAZZIO, GUSTAVO M. DALPIAN, Universidade Federal do ABC — Spintronic has a particular interest in diluted magnetic semiconductors because these materials present both semiconducting and magnetic properties at the same time. ZnO-based materials and nanostructures have potential applications in this area because they can present room-temperature ferromagnetism when doped with transition metals and, in some cases, spin polarization can be observed even without magnetic impurities. Following recent experimental results reporting this [Nano Lett. 6, 1489 (2007)], we have analyzed several ZnO nanocrystals, with diameters varying from 0.9 to 1.78 nm. Using DFT, we observed that a large amount of surface reconstructions appear in the non-passivated nanocrystals. Depending on the reconstruction, spin polarization without magnetic impurities can be observed at the surface region, what can lead to long-range spin interactions. Thus, we propose that the referred experimental results for nanostructured ZnO can be originated by extended defects such as surfaces. This can also explain the same magnetic behavior presented by non-doped thin films and other ZnO nanostructures.

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Aline L. Schoenhalz
Universidade Federal do ABC

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