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Dimensionality and stoichiometry effects on magnetic properties of Fe_xCo_{1-x} nanostructures on Pt(111) from first principles[1] HELENA PETRILLI, IVAN MIRANDA, Instituto de Física, Universidade de São Paulo, Brazil, RICARDO IGARASHI, Escola de Engenharia e Tecnologia, Universidade Anhembi Morumbi, Brazil, ANGELA KLAUTAU, Faculdade de Física, Universidade Federal do Pará, Brazil — We investigate the influence of dimensionality and stoichiometry changes on the behavior of local magnetic moments and exchange coupling parameters of Fe_xCo_{1-x} nanostructures deposited on the fcc Pt(111) surface. The electronic and magnetic structures of these Fe_xCo_{1-x}/Pt(111) systems are studied using the first-principles RS-LMTO-ASA method in the framework of the DFT. We consider different configurations of linear-shaped or compact-shaped trimers and heptamers, varying the internal positions and the concentration of Fe or Co atoms. The existence of a strictly decreasing nonlinear trend of the average orbital moments with the Fe concentration for the compact clusters is demonstrated, and differs from what was found for higher-dimensional Fe_xCo_{1-x} systems (monolayer/Pt(111) and bulk). Although all studied linear and compact Fe_xCo_{1-x} configurations have shown to be substancially ferromagnetic between nearest Fe or Co neighbors, not all revealed a collinear ground state, presenting, in some cases, oscillating exchange parameters for further distances and a non-negligible Dzyaloshinskii-Moriya interaction, induced by the Pt strong spin-orbit coupling.

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