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First Principles Theory of Supported Clusters with Complex Magnetic Order.

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It is demonstrated that the magnetic interactions can be drastically different for nano-sized systems compared to those of bulk or surfaces. In a real-space formalism we have developed a technique to calculate non-collinear magnetization structures and hence exchange interactions. Our results for magnetic Cr, Mn and Fe clusters supported on a Cu(111) surface show that the magnetic ordering as a rule is non-collinear and can not always be described using a simple Heisenberg Hamiltonian. We argue that the use of *ab initio* calculations allowing for non-collinear coupling between atomic spins constitute an efficient and reliable way of analyzing nano-sized magnets.