

Fall 2009 Colloquia

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Magnetic nanostructures coupled to environments

Due to recent advances in fabrication and measurement techniques, new magnetic nanostructures can be synthesized and their quantum properties can be locally probed at the molecular level. Despite this progress, it still remains challenging to characterize interfaces and contacts and to manipulate their properties for specific applications. A understanding of such properties requires theoretical models as well as large-scale computer simulations considering local environmental factors at the atomistic level. Recently, low-dimensional structures made of nanoscale magnetic molecules have drawn attention due to its unique interplay between the internal magnetic degrees of freedom and electronic ones and to possible applications for information storage and materials for quantum computation. In this talk, we consider a monolayer of such magnetic molecules adsorbed on a metallic surface and a single magnetic molecule bridged between electrodes that have been recently synthesized.

We discuss how the electronic, magnetic, and transport properties of the magnetic molecules are influenced by the interactions with the surface or the electrodes, using simulations based on first-principles methods.

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