The interaction between a molecular magnet monolayer and a metallic surface

Salvador Barraza-Lopez, Michael C. Avery and Kyungwha Park

Department of Physics, Virginia Tech
Blacksburg, VA, USA

Over the past decade, molecular magnets or single-molecule magnets have drawn considerable attention due to observed magnetic quantum tunneling and interference and the possibility of using them for information storage or devices. There have been so far significant efforts to build and characterize thin films or monolayers of single-molecule magnets on surfaces or single-molecule magnets bridged between electrodes. However, there is the need to understand changes of the properties of single-molecule magnets in those environments using atomic-scale simulations. In this regard, we simulate, within density-functional theory, a nanostructure in which prototype Mn_{12} molecules are adsorbed via a thiol group onto a gold surface.[1,2] Based on a supercell calculation, we investigate how much charge and spin are transferred between a Mn_{12} molecule and the metal surface. In addition, we will compare the electronic structure and magnetic properties of the nanostructure with those of an isolated Mn_{12} molecule in the absence and presence of spin-orbit interaction. Financial support was provided by the Jeffress Memorial Trust Funds and computational support by the National Center for Supercomputing Applications.

[1] S. Barraza-Lopez, M. C. Avery, and Kyungwha Park, "First-principles study of a single-molecule magnet Mn12 monolayer on the Au(111) surface," Phys. Rev. B **76**, 224413 (2007).

[2] S. Barraza-Lopez, M. C. Avery, and Kyungwha Park, "Interaction between a monolayer of single-molecule magnets and a metal surface," J. Appl. Phys. **103**, 07B907 (2008).