MAR11-2010-002006

Abstract for an Invited Paper
for the MAR11 Meeting of
the American Physical Society

Electronic Structure and Transport Through Single Molecule Magnets[1]

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Over the past decade, single-molecule magnets have drawn considerable attention due to observed magnetic quantum tunneling and interference and a possibility of using them for information storage or devices. There have been so far significant experimental efforts to build and characterize monolayers of single-molecule magnets on various surfaces or single-molecule magnets connected to electrodes. There is need to understand changes of electronic and magnetic properties of single-molecule magnets in those environments using quantum mechanical simulations. We simulate, within density-functional theory, a nanostructure in which prototype single-molecule magnets Mn12 are adsorbed onto a gold surface. We investigate coupling between the Mn12 and the surface and discuss electronic structure and magnetic anisotropy of the Mn12 on a gold surface in comparison to an isolated Mn12. In addition, we present electron transport properties through a Mn12 bridged between gold electrodes, using the nonequilibrium Green's function method in conjunction with density-functional theory. We discuss a possibility of using a Mn12 molecule as a spin filter and an effect of interface geometry and bonding type on transport across a Mn12.

[1]Supported by NSF DMR.