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First-principles study of a monolayer of single-molecule magnets Mn_{12} on a gold surface SALVADOR BARRAZA-LOPEZ, MICHAEL C. AVERY, KYUNGWHA PARK, Department of Physics, Virginia Polytechnic Institute and State University, Blacksburg VA, 24061 — 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 in devices. There have been significant experimental efforts to build and characterize thin films or monolayers of single-molecule magnets on surfaces or single-molecule magnets bridged between electrodes. In parallel, theoretical models have been proposed to understand the properties of single-molecule magnets coupled to a metal substrate. However, there do not exist atomic-scale simulations on this complex system. We simulate, within density-functional theory, prototype Mn_{12} molecules adsorbed via a thiol group onto a gold surface. We investigate how strongly a Mn_{12} molecule is coupled to the metal surface and how much charge and spin moments are transferred between a Mn_{12} molecule monolayer and the metal surface. In particular, we compare the electronic and magnetic properties of the Mn_{12} monolayer on a gold surface with those of an isolated Mn_{12} in the presence of spin-orbit interaction. Our results may shed light into tailoring of the magnetic properties of nanomagnets as a result of electronic transfer from a proximal metallic surface.

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