First-principles study of substrate effects on electronic and magnetic properties of lanthanide-based single-molecule magnets

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Lanthanide-based single-molecule magnets (SMMs) have been shown to be more stable in the experimental fabrication of monolayers or single-molecule transistors than 3d transition metal-based SMMs. Recently, various types of lanthanide-based SMMs have been synthesized with their properties manipulated by varying the attached ligand structure. Single-molecule transistors based on lanthanide SMMs have shown control of molecular nuclear spins by an electric field, which has a potential application for quantum information. Here we investigate electronic and magnetic properties of an isolated Terbium(III) Bis-phthalocyaninato ($TbPc_2$) SMM in neutral and charged states and external perturbations. Furthermore, we explore the effects of the substrate on these properties. We use density-functional theory with on-site Coulomb repulsion terms for the Tb f orbitals. We also compare our calculated results with existing experimental data.

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