

Abstract Submitted
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A first-principles study of a single-molecule magnet Mn12 adsorbed on Bi(111)¹ KYUNGWHA PARK, Department of Physics, Virginia Tech, Blacksburg, VA 24061, USA, JUN-ZHONG WANG, School of Physical Science and Technology, Southwest Univ., Chongqing 400715, China — Recently, elemental Bi and Bi-based alloys have attracted a lot of attention due to unique quantum properties of their surface states induced by strong spin-orbit coupling. A single-molecule magnet Mn12 is known to be a prototype molecular magnet with significant magnetic anisotropy caused by spin-orbit coupling. Despite a great effort to fabricate monolayers of single-molecule magnets on various substrates, there are few studies of single-molecule magnets on strongly spin-orbit coupled substrates. Here we present our theoretical study of electronic and magnetic properties of single-molecule magnets Mn12 adsorbed on a strongly spin-orbit coupled semi-metallic Bi surface without any linker molecules. This work was motivated by a recent low-temperature scanning tunneling microscopy (STM) experiment where individual single-molecule magnets Mn12 were grafted on Bi. We apply density-functional theory (DFT) including on-site Coulomb repulsion U and self-consistent spin-orbit coupling, to two adsorption geometries of Mn12 on Bi. We compare our calculated electronic and magnetic properties of the Mn12 molecule on Bi with those of an isolated Mn12.

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