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Effects of bonding type and interface geometry on coherent transport through the single-molecule magnet Mn12[1] KYUNGWHA PARK, Virginia Tech, SALVADOR BARRAZA-LOPEZ, Georgia Tech, VICTOR GARCIA-SUAREZ, Lancaster University, UK, JAIME FERRER, University of Oviedo, Spain — We investigate coherent electron transport through the single-molecule magnet Mn12, connected to Au electrodes, using the nonequilibrium Green's function method and density-functional theory. We analyze the impact on the electronic properties, and charge and spin transport across the junction of (i) using different bonding mechanisms and linker molecules; (ii) letting the geometry of the junction relax; (iii) using different molecular orientations. We consider nine interface geometries leading to five different bonding mechanisms and two molecular orientations. The two molecular orientations of Mn12 considered correspond to the magnetic easy axis of Mn12 parallel or normal to the direction of the electron transport. The general trend among the different bonding types and molecular orientations obtained from this study may be applied to transport through other single-molecule magnets.

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