DFT studies on double-decker phthalocyaninato-Tb complex

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Abstract

Electronic structure and molecular structure of the double-decker phthalocyaninato(Pc)-Tb complex are investigated by the DFT method. In order to clarify which functional set and basis set are appropriate for the quantitative study, several combinations of these sets are comparatively examined. The spin structures of *f*-electrons and spin distributions are also discussed to describe the magnetic properties of the complex.