A Haldane-Anderson model study for the iron spin and charge state in Myoglobin

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Heme metalloproteins are responsible for some of the most important biological process of life such as respiration and energy production. Their biological activity is known to be determined mostly by the spin state of the transition metal ions located in the center of their active sites[1] Various quantum chemical *ab initio* methods based on the density functional theory (DFT) have been used to better understand the relation between the spin state and the protein functionalities. However, it is well known that the DFT-based methods often predict the electronic states of transition metals which are not consistent with experimental observations.[2] In this work, we propose a new approach to study the spin and charge states of the transition metal ions in metalloproteins. First, using standard DFT calculations, we construct a tight binding model Hamiltonian coupled to the transition metal ions. Next, we solve the model using various numerical methods developed recently in the field of strongly correlated electrons. We shall demonstrate our new approach applied to Myoglobin, one of the simplest metalloprotein.

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