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Controlling Spin State of Magnetic Molecules by Oxygen Binding Studied Using Scanning Tunneling Microscopy SOON-HYEONG LEE, Korea University, YUN HEE CHANG, KAIST, HOWON KIM, KYUNG MIN KIM, Korea University, YONG-HYUN KIM, KAIST, SE-JONG KAHNG, Korea University — Binding and unbinding between molecular oxygen and metallo-porphyrin is a key process for oxygen delivery in respiration. It can be also used to control spin state of magnetic metallo-porphyrin molecules. Controlling and sensing spin states of magnetic molecules in such reactions at the single molecule level is essential for spintronic molecular device applications. Here, we demonstrate that spin states of metallo-porphyrin on surfaces can be controlled over by binding and unbinding of oxygen molecule, and be sensed using scanning tunneling microscopy and spectroscopy. Kondo localized state of metallo-porphyrin showed significant modification by the binding of oxygen molecule, implying that the spin state was changed. Our density functional theory calculation results explain the observations with the hybridization of unpaired spins in d and π^* orbitals of metallo-porphyrin and oxygen, respectively. Our study opens up ways to control molecular spin state and Kondo effect by means of molecular binding and unbinding reactions on surfaces.

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