Externally controlled spin state switching in metal-organic complexes. ALEXEI BAGRETS, VELIMIR MEDED, MARIO RUBEN, FERDINAND EVERS, Institute of Nanotechnology, Research Center Karlsruhe, Germany — Recent transport experiments have demonstrated that a manipulation of the charge of individual molecules is feasible using electromigrated metal junctions [1] or electrochemical gates in conjunction with the STM [2]. Using elaborated density functional theory calculations, we will discuss a possibility to induce — by means of charging or applied stress — a switching between low and high spin states in certain metal-organic systems, \([\text{Fe(bpp)}_2]^{2+}\) (bpp: bispyrazolyl pyridine) and \([\text{Mn(tpy)}_2]^{2+}\) (tpy: terpyridine). Based upon a recent success of the single molecular conduction experiment through Ru(II) complex [3], we anticipate the transport properties of Fe(II) and Mn(II) complexes to be gate controlled via exploiting their spin degree of freedom.


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