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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, $[Fe(bpp)_2]^{2+}$ (bpp: bispyrazolyl pyridine) and $[Mn(tpy)_2]^{2+}$ (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.

[1] E. A. Osorio *et al.*, J. Phys.: Condens. Matter**20**, 374121 (2008); [2] F. Chen *el al.*, Ann. Rev. Phys. Chem. **58**, 535 (2007); Li *et al.*, Nanotechnology **18**, 044018 (2007). [3] M. Ruben, A. Landa, E. Lörtscher, H. Riel, M. Mayor, H. Görls, H. Weber, A. Arnold, and F. Evers, Small (online), DOI: 10.1002/smll.200800390 (2008).

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