

Abstract Submitted  
for the MAR08 Meeting of  
The American Physical Society

***Ab initio* simulations of the transport properties of Mn<sub>12</sub> based spin-devices** CHAITANYA DAS PEMMARAJU, IVAN RUNGGER, STEFANO SANVITO, Trinity College Dublin, Ireland, COMPUTATIONAL SPINTRONICS GROUP, TCD TEAM — Single-molecule magnets (SMMs) represent a unique playground for fundamental quantum physics and exhibit exotic phenomena such as magnetic hysteresis as well as magnetization reversal through quantum tunneling. Recently, transport measurements on Mn<sub>12</sub> based molecular magnets in single-molecule-transistor devices have been realized. In this work we present *ab initio* transport[1] calculations of Mn<sub>12</sub> molecules functionalized by thioether groups and sandwiched between gold contacts. We find the transport properties of these SMMs to be dominated by tunneling type behaviour across the organic functional groups and asymmetric coupling to the leads. We observe asymmetric I-V curves under positive and negative bias. In addition we demonstrate that the I-V characteristic changes upon changing the magnetic state of the molecule, suggesting that electrical single-spin detection can be indeed obtained from a detailed knowledge of the I-V. [1] Rocha *et. al*, Spin and Molecular Electronics in an Atomically Generated Orbital Landscape; URL: <http://www.smeagol.tcd.ie>

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Date submitted: 18 Dec 2007

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