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Effect of strong correlations on the electronic and transport properties of porphyrin wires[1] VICTOR MANUEL GARCIA SUAREZ, Departamento de Fisica, Universidad de Oviedo AND CINN (CSIC) AND Physics Department, Lancaster University, RUBEN FERRADAS, Departamento de Fisica, Universidad de Oviedo AND CINN (CSIC), JAIME FERRER, Departamento de Fisica, Universidad de Oviedo AND CINN (CSIC) AND Physics Department, Lancaster University, THEORY GROUP, CONDENSED MATTER TEAM — Recent transport experiments performed on porphyrin molecules show that wires based on these molecules could be used to design future nanoscale elements with low attenunation as a function of distance and able to work at room temperature. Apart from their rather good transport properties, which come from the conjugation of their molecular backbone, porphyrins are also very interesting due to the fact that they have a metallic element in the middle that affects their electronic properties and could also introduce magnetic effects. In this talk I will show first-principles simulations based on density functional on the electronic and transport properties of porphyrin wires between gold leads, paying special attention to the effect of using different metallic elements in the central part of the molecule (Fe, Co, Ni, Zn and Cu). Strong correlations are introduced in the form of LDA+U. The results show that the metallic element plays a crucial role in the electronic structure of the molecule around the HOMO and LUMO orbitals and introduces magnetic effects that affect the transport properties.

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