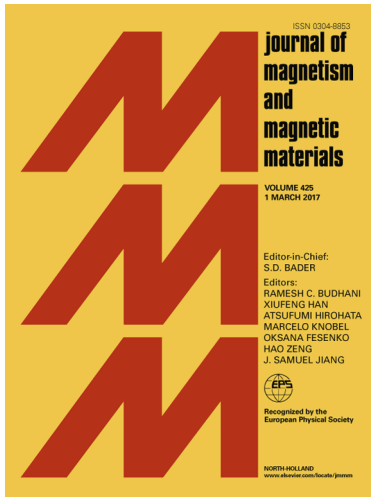

Possibility of a Ferromagnetic and Conducting Metal-Organic Network

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PII: S0304-8853(17)32559-3
DOI: https://doi.org/10.1016/j.jmmm.2018.01.005
Reference: MAGMA 63583

To appear in: *Journal of Magnetism and Magnetic Materials*

Received Date: 15 August 2017
Revised Date: 29 November 2017
Accepted Date: 2 January 2018

Please cite this article as: M. Mabrouk, R. Hayn, H. Denawi, R. Ben Chaabane, Possibility of a Ferromagnetic and Conducting Metal-Organic Network, *Journal of Magnetism and Magnetic Materials* (2018), doi: https://doi.org/10.1016/j.jmmm.2018.01.005

Possibility of a Ferromagnetic and Conducting Metal-Organic Network

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Abstract

In this paper, we present first principles calculations based on the spin-polarized generalized gradient approximation with on-site Coulomb repulsion term (SGGA+*U*), to explore the electronic and magnetic properties of the novel planar metal-organic networks TM-Pc and TM-TCNB (where TM means a transition metal of the 3*d* series: Ti, V, Cr, ..., or Zn, Pc - Phthalocyanine, and TCNB - Tetracyanobenzene) as free-standing sheets. This work is an extension of two earlier research works dealing with the Mn (M. Mabrouk et al., Phys. Rev. B: Condens. Matter Mater. Phys. 92 (2015) 184424) and Fe (M. Mabrouk et al., J. Phys. Chem. C 121 (2017) 4253) cases. Our theoretical investigations demonstrate that TM-Pc are more stable than TM-TCNB. Our results unveil that all the TM-Pc frameworks have an insulating behavior with the exception of Mn-Pc which is half-metallic and favor antiferromagnetic order in the case of our magnetic systems except for V-Pc which is ferromagnetic. In contrast, the TM-TCNB networks are metallic at least in one spin direction and exhibit long-range ferromagnetic coupling in case for magnetic structures, which represent ideal candidates and an interesting prospect of unprecedented applications in spintronics. In addition, these results may shed light to achieve a new pathway on further experimental research in molecular spintronics.

Keywords: Ab-initio calculations; DFT+*U*; Magnetism; Pc; TCNB.

1. Introduction

Recently, tremendous effort has been devoted to experimental or theoretical studies of two-dimensional (*2D*) artificial metal-organic nanostructured materials in further development of graphene [1, 2]. They have an enormous range of possible applications, ranging from catalysis over gas- or biosensing, photodynamic therapy up to spintronics. In light of the latter application, especially nanostructured magnetic memory devices are discussed. To reach the