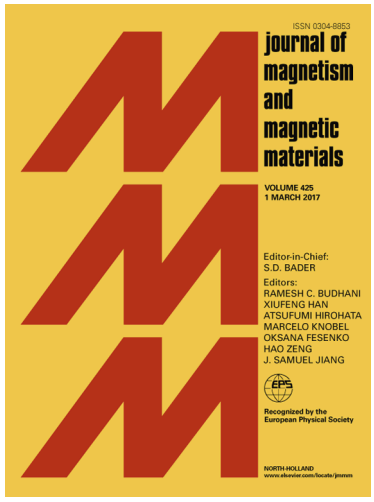

Magnetization on nitrogen in extended honeycomb carbon layers from first principles: Case studies of CxN (x = 2, 6, 12)

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Abstract.

Identification of unusual onset of spin polarization of N(*p*) states is reported. Full saturation up to $3\mu_B$ (Bohr Magnetons) is demonstrated within extended two-dimensional carbon networks of C_xN (x= 2, 6, 12) hexagonal structures refined based on density functional theory calculations. The cohesive energy is found to increase along the extension of the carbon network which opens perspective to experimental investigations through reactive deposition of thin films. Establishing the energy-volume equations of states of the two carbon rich nitrides done with assuming spin degenerate (non spin polarized) and spin-polarized configurations, the ground state is identified as ferromagnetic in both C_6N and $C_{12}N$. The electronic density of states show vanishing intensities at the Fermi level, whence the integer magnetizations. The variation of magnetization with volume points to strongly ferromagnetic behavior.

I- Introduction

The occurrence of magnetic spin polarization such as in the three ferromagnetic transition metals: Fe, Co and Ni requires a significant localization of the states carrying the finite magnetic moment, here the electrons in the 3d subshell –that can be identified in calculations– by a high density of states (DOS) at the Fermi level $n(E_F)$ in an initially total spins electronic system.

Quantitatively, $n(E_F)$ is obtained thanks to quantum physics calculations within the well established framework of the density functional theory DFT [1,2] and inferred from the Stoner theory of band (ferro)magnetism [3]. Then the localization of states leading to a large $n(E_F)$ magnitude is an indication of energetically unstable electronic system in spin degenerate configuration (also labeled non spin polarized NSP) and that it should lowers its energy by spin polarization (SP) via a redistribution of the electrons into two spin populations: ↑ usually labeled as "majority spins" (larger number of electrons) and ↓ labeled as "minority spins" (smaller number of electrons). The difference between ↑ and ↓ spin populations gives a finite magnetic moment.

In general magnetization develops on n*d* states of transition metals or n*f* states of rare-earths and actinides: n*f* (n = 4, 5 respectively). Regarding transition metals n*d* (*n* = 3, 4, 5), the first period (*n* = 3) developing finite magnetization are ferromagnetic metals Fe, Co and Ni, but not metals of 2nd (*n* = 4) and 3rd (*n* = 5) periods because their 4*d* and 5*d* bands are too broad to allow for *d* states to localize enough. Also rare earth Gadolinium is a ferromagnet at room temperature with M= $7\mu_B$ magnetic moment. Note that while in 3*d* ferromagnetic metals the