Role of dopants in tuning spintronic features of lithium doped g-C_4N_3@$Li_{n\ =1\ to\ 4}$

Role of dopants in tuning spintronic features of lithium doped g-C_4N_3@$Li_{n=1\ to\ 4}$

Shankar Prasad Mitra[1], Ajit Biswas[1], Souradip Dey[2], Utsab Roy[3], Rinki Bhowmick[1], Mausumi Chattopadhyaya[4], Tanmoy Dutta[5], Jit Chakraborty[5] and Sabyasachi Sen[1*]

[1]Department of Physics, JIS College of Engineering, Kalyani, Nadia, PIN- 741235, India.
[2]Department of MCNT, JIS College of Engineering, Kalyani, Nadia, PIN- 741235, India.
[3]Department of Bio-Medical Engineering, JIS College of Engineering, Kalyani, Nadia, PIN-741235, India.
[4]Department of Chemistry, NIT, Calicut, Calicut Mukkam Road, Kattangal, Kerala, 673601.
[5]Department of Chemistry, JIS College of Engineering, Kalyani, Nadia, PIN- 741235, India.
*sabyaphy12@gmail.com.

Abstract. We report herein, charge transfer assisted tuning of electronic and spintronic feature of g-C_4N_3@$Li_{n=1-4}$ systems. Complete removal of spintronic feature is observed at the doping concentration 14.28%. At lower doping concentration, half metallic feature is observed with clear manifestation of negative differential resistance, which is predominant at n=3. We also noticed significant modifications in current-voltage characteristics as the number of dopants flips from odd to even numbers. Observed feature is mainly attributed to increased charge transfer from Li atom to the g-C_4N_3 backbone at higher doping concentration and concomitant enhancement in electron-electron interactions. These observations are in corroboration with molecular orbital picture obtained at various doping concentrations.

1. Introduction

In the last two decades enormous research attention has been shown in the emerging field of spin dependent electronics or spintronics where the electronic spins are exploited as an extra degree of freedom in addition to electronic charge. In spintronics, digital data can be stored and transferred efficiently with low power consumption [1]. Thus the phenomenon of spintronics provides a new window in the field of quantum computing. To develop spintronics materials half-metallicity and metal-free magnetism are the two foremost and fundamental properties that should be emphasised [2, 3]. A half metal is characterized with the generation of spin-polarized current i.e. it behaves like a metal in one spin channel and semiconductor in the other so it has an ability to filter the current into a single spin channel around Fermi level.

In the recent past experimental exploration of metal-free half-metal was a real challenge. Eventually such a promising material known as graphitic carbon nitride (g-C_4N_3) has been successfully synthesized [4]. The naturally occurring molecule C_3N_4 reconstructed into a 2 dimensional structure known as g-C_3N_4 with natural vacancies existing in its 2x2 layer. Several research reveals that in bulk g-C_3N_4 is non-magnetic in nature [5, 6]; whereas another very similar 2-dimensional structure was synthesized in the framework of g-C_3N_4 named as graphitic carbon nitride (g-C_4N_3) with an extra carbon doped outside the ring (figure 1), shows half metallic features [4] and ferro magneticity [7]. It is believed that magnetic property arises due to the presence of transition materials having partially filled 3d electrons though