



# Role of d-orbital electrons in tuning multifunctional spintronic action in pi-stacked $C_n-C_6H_6-Fe-C_6H_6-C_{13-n}$

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## ABSTRACT

We report here in emergence of intriguing spintronic actions in  $\pi$  stacked complex  $C_n-C_6H_6-Fe-C_6H_6-C_{13-n}$ , while sandwiched between two Fe(100) electrodes. The system shows notable spin rectification ratio of 4.23 at  $n = 2$  and manifests spin filtration at  $n = 4$ . Observed multifunctionality of this single molecule with varying spacer length was explained by analysing the density of states, transmission coefficients of tunneling electrons and probability wave interpretation through Molecular Projected Self-Consistent Hamiltonian States. Interestingly, we found that in spite of the presence of Fe 3d orbitals, the device property is mainly channelised through the 2p orbital of C atoms. The present investigation emphasises that the salient spintronic feature can be modulated simply by varying the spacer length without altering the metal site.

## 1. Introduction

Scavenging suitable material exhibiting novel spintronic behavior has been identified as one of the major areas of concern of modern day nanoelectronic device design. Within spintronics, in addition to charge transport; change in spin state of an electron is exploited to carry the information and such devices are contributing to ultra edge technological revolutions form logic gates in quantum computer to efficient memory devices [1]. This elegant performance of spintronic devices emerges due to large spin-coherence time, less power dissipation and availability in various organic conformations [2–9]. This supremacy of the spintronic devices over its charge counterpart has been reported in a number of literatures [10–17] and majority of them potrayaed spin filtration, spin valve action, spin switching, spin transfer torque action as efficient exhibition of spintronic action. In most of the hitherto reported literatures the emergence of spintronic feature is reported to be mediated by the ferromagnetic metals having significant contributions from d-electrons either from molecular part or from the electrode part or both. Albeit there are precedence of metal free magnets but in respect of versatile applicaitons like single molecular magnet to spin qubit generation of quantum circuit; presence of d-electron centre certainly plays a pivotal role. Keeping this fact in mind we have preferred a system having one ferromagnetic centre in a pi-stacked  $SC_n-C_6H_6-Fe-C_6H_6-$

$C_{13-n}-S$  (where  $n = 2,4$ ) sandwiched between two magnetic Fe (100) electrodes and examined the role of d-electrons in determining overall spintronic feature of the system.

In molecular electronics, spin rectification is an extremely important device applications and the underlying physics behind rectification in such devices is attributed to spatial asymmetries evident in the asymmetric current ( $I$ )-voltage ( $V$ ) characteristics with  $I(-V) \neq I(V)$ , where  $I$  denotes the electric current in presence of an external bias  $V$ . At the molecular level current rectification are mainly categorised as (i) *extrinsic* and (ii) *intrinsic* rectifier. Binding between asymmetric molecule-electrode or usage of different materials as source or drain electrodes are the examples of the first kind. *Intrinsic* rectifiers utilizes the in-built asymmetry in the molecular structure, e.g. an asymmetric diblock co-oligomer. Spin rectification in molecular systems have been reported in a number of literatures including the rudimentary invention of Dalglish and Kirzenow [1]. They reported spin rectification action in organic molecule coupled with one ferromagnetic and one nonmagnetic metal and the spatial spin asymmetry was contributed by the external electrodes. Khymyn et al. [18] reported spin rectification on a system of AFM dielectric with bi-axial crystallographic anisotropy (e.g., NiO). Length dependence of spin-rectification was reported by Gui-Chao Hu et al. [19] and they found both spin and charge current rectification for different lengths. Zbigniew and coworkers [20] observed

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