# CHARGE TRANSPORT IN MOLECULAR MAGNETO NANOELECTRONIC DEVICES

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Shaping the properties of matter at the nanoscale to realise electronic devices is the vision of *nanoelectronics. Molecular spintronics* thus emerges as a growing research field at the frontier of *nanoelectronics* where electronic magnetic and mechanical properties of single molecules, assemblies of molecules, and crystals of molecules are studied systematically aiming at successful miniaturisation of electronic devices down to the nanoscale. However to build an electronic circuit entirely at the molecular level is quite challenging, due primarily to complexities with the molecular conformations electrode topology and nanoscale interconnects. It has been observed that the molecular conformation, as well as the ferromagnetic electrode molecule coupling, can powerfully impact the interfacial spin properties from the spin polarisation enhancement to its design-control in *nanodevices*. However, an exciting challenge remains in finding opportunities to develop new spintronic functionalities and new spintronic devices with unique quantum properties.

Though there have been considerable signs of progress on the experimental as well as the ideal font for analysing the quantum transport properties at the nanoscale intricacies still exit considerably when it comes to a comprehensive understanding of the underlying mechanism behind various interactions within devices. Our proposed work in this thesis would hence be aiming at dynamic modelling of spin-polarised quantum transport from *first principles* and following prediction of new spintronic functionalities to potentially facilitate better designing of future *nanodevices*. From the *nanodevice* point of view, the use of *organic* and *organo-metallic* molecular junctions has been explored simultaneously.

These investigations provided predictions of recent quantum transport behaviour modelling of devices in different molecules that will drive future analysis towards their experimental realisation of molecular *nanoelectronic* and *spintronic devices*.

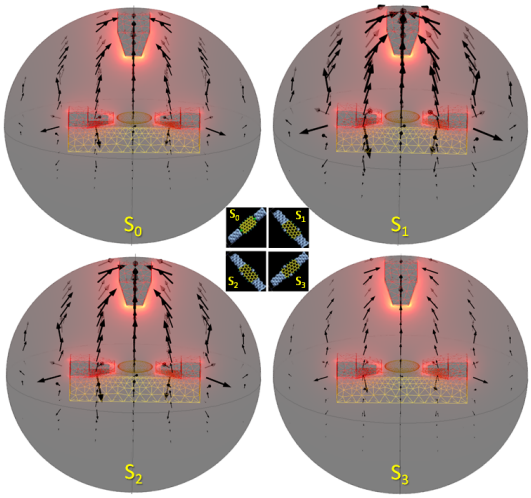



**Figure 1:**Shows the COMSOL Multiphysics simulation results for the designed three electrode model using electrostatic physics model. Potential distribution across undoped and doped z-GND junctions at different dopant sites $S_1$,$S_2$,$S_3$,$S_4$ in which the $S_1$ site has the high potential distribution across the nano-junction which can act as single electron transistors.