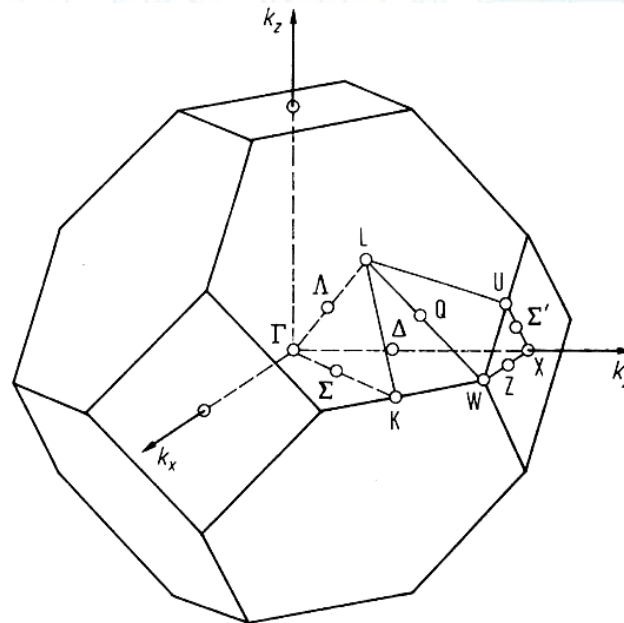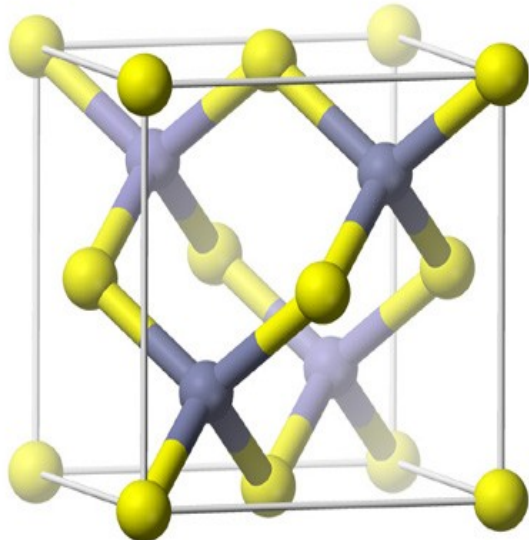# Magnetic Semiconductors

Ryky Nelson

Advisors: Juana Moreno, Mark Jarell
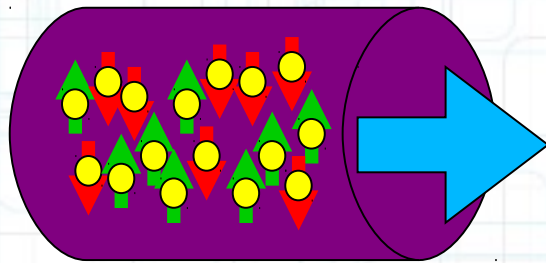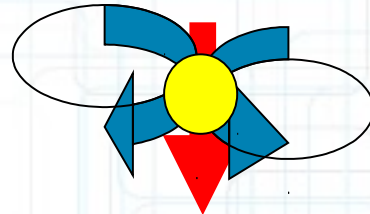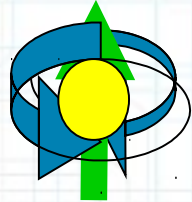**Louisiana State University**

What am I doing?

- To model Magentic Semiconductors
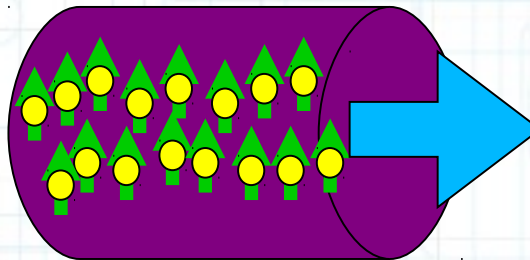- Presently, to model conventional semiconductors
- GaAs & GaN

- GaAs & GaN are dilutely doped by magnetic atoms

- Impurty atoms: Manganese

Why Magnetic Semiconductors?

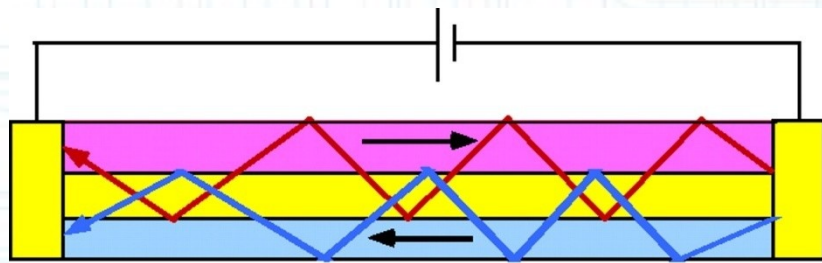- Spin and charge degrees of freedom are coupled each other.
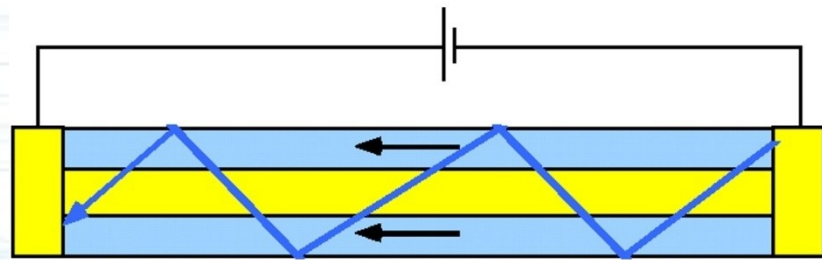

Spin-unpolarized currents
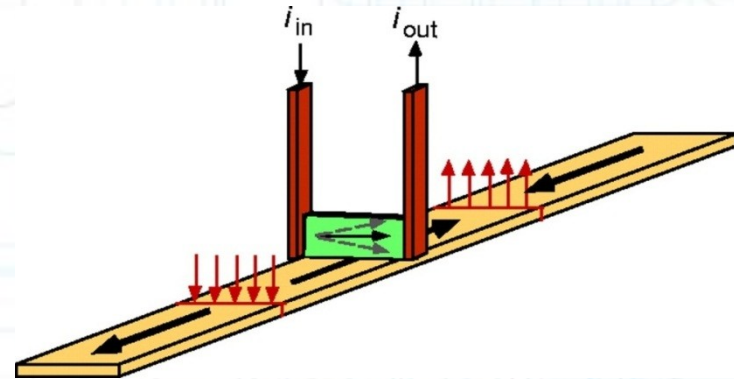
Spin-polarized currents

- A good candidate for spintronic materials.
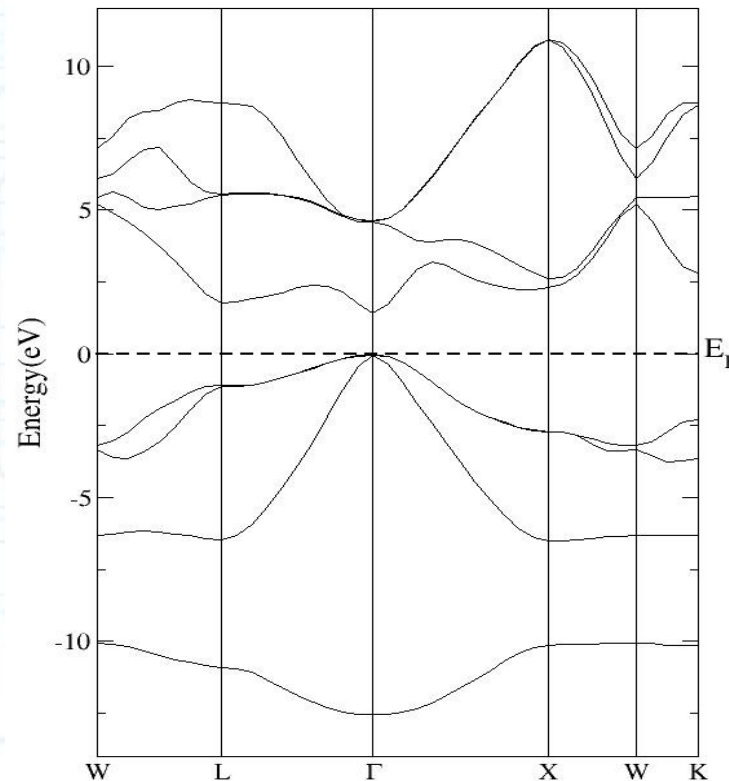

High resistance

Low resistance

i_{in} i_{out}

How do we model our systems?

- Using DFT and a Wannier-function-based downfolding method to get an effective Hamiltonian, H_0, for the host crystals: GaAs & GaN
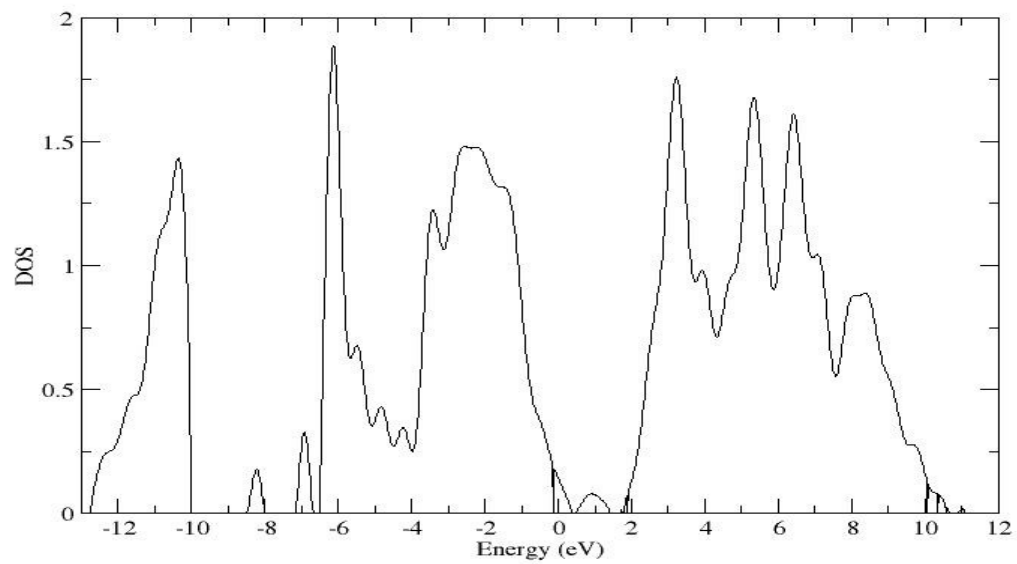
- Adding the double exchange interaction H1 due to interaction between local spins Mn mediated by carriers.

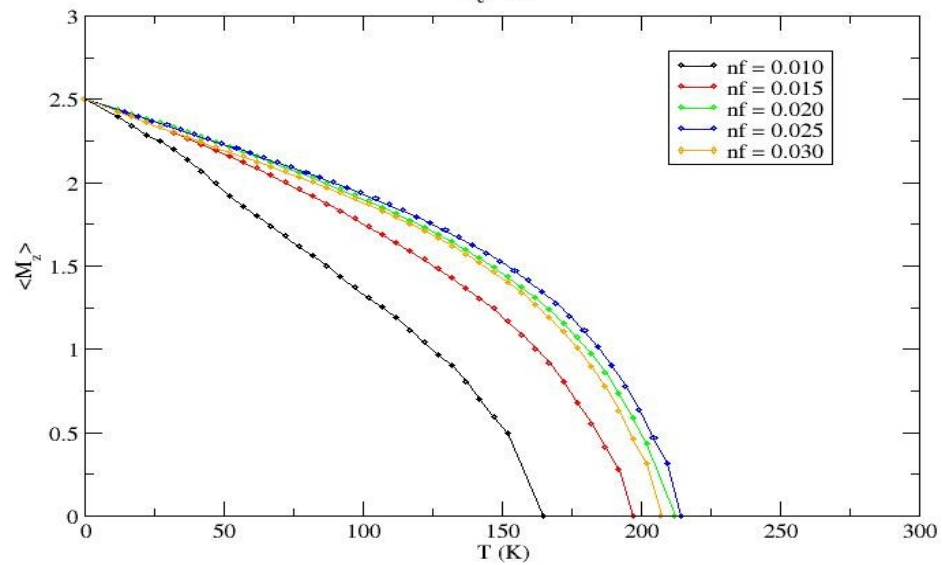$$H1 = -J \sum_i \vec{S}_i \cdot \vec{\sigma}$$

- The magnetic and electric properties are calculated using Dynamical Mean Field Approximation self-consistently and numerically.
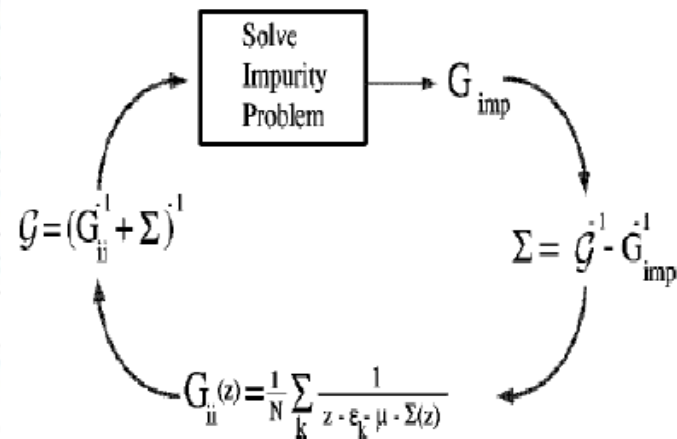
The DMFA algorithm

Magetization Vs T

$J_c = 2.0$

Where do we perform our numerical?

- We use Kraken Cray XT5 high performance computers at NICS

- We implement Message Passing Interface (MPI) to parallel our code and to make our calculation finished faster.

- The number cores up to 360 cores

- The run-time 60 -180 minutes

- The problem exists when we have many jobs to run and require big resources.

- We are about to implement manyjob and Bigjob to tackle the problem

Future Work

- To model organic semiconductors
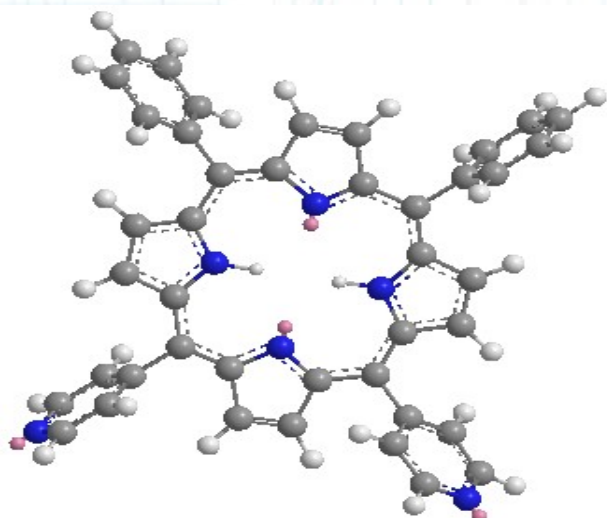
- A porphyrin is a heterocyclic aromatic ring made from 4 pyrrole subunits (C4NH5) joined on opposite sides through 4 methine links.

- The central cavity allows for magnetic atoms to be inserting conferring metalloporphyrins very interesting magnetic properties.

Acknowledgement

THANK YOU