FZU: DFT Calculattions

many

March 2024

1 Tasks

:

- Check the convergence of the ground state energies for the uu nn dd (ferrimagnetic), ud nn ud (antiferromagnetic) and uu nn uu (ferromagnetic) configuration with respect to the number of k-points. (LDA and GGA)

- Plot please E(#k), M(#k) t(#k)!

- Extract the minimum necessary k-points.

1.1 Calculate Ground state energies and magnetic momenta for the following configurations and the LDA and GGA functionals:

(see Table 1)
   Nice sticks and balls plots with magnetic momenta depicted?

1.2 Only once (?)

1. DOS: calculate DOS for GGA and LDA (ferrimagnetic)

2. DOSplot for each and Δ DOS

3. Analyse convergence of each run and try to identify "suspicious" runs.?

	LDA				
	Energy	mag. Moment	ΔE [mRy]	Energy	mag
uu nn dd (ferrimagnetic)	-35164.84355323	-2.34662	0	-35203.71313403	
ud nn ud	-35164.82028797	0.00006	23.26526	-35203.68222677	
ud nn du	identical to ud nn ud				
du nn ud					
du nn du					
uu nn uu (ferromagnetic)	-35164.81576070	12.27372	27.7925299961	-35203.68793386	
dd nn dd (ferromagnetic)					

Table 1: Overview of necessary runs. Use the (suposedly converged) k-point number extracted above. ΔE refers to the energy difference of each configuration to the ground state energy of the respective lowest configuration in energy. For GGA we expect the ferrimagnetic configuration to be the lowest in energy and $\Delta E = 15 mRydberg$ for ud nn ud (AFM 1).