Search for High Magnetization (FeCo and $Fe_{16}N_2$)

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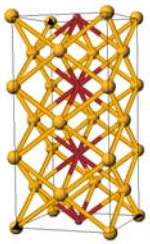
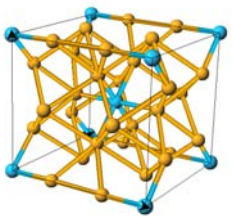
FeCo and $Fe_{16}N_2$

The search for higher magnetization derives from the need for magnetically soft materials possessing high magnetic moments. A very common such material is FeCo, which is at the maximum of the Slater-Pauling curve. Much less common is $Fe_{16}N_2$, for which we examine the possibility of substantiation of reported ultra-high moments. All calculations are done using VASP (Vienna ab-initio simulation package).

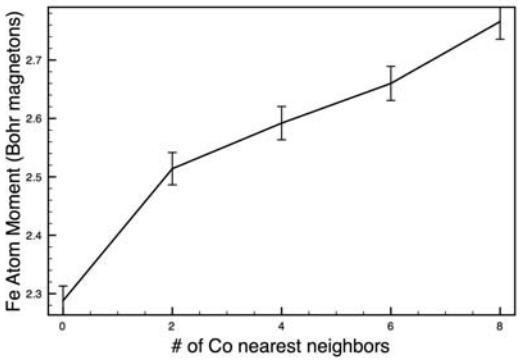
bcc FeCo



bct $Fe_{16}N_2$

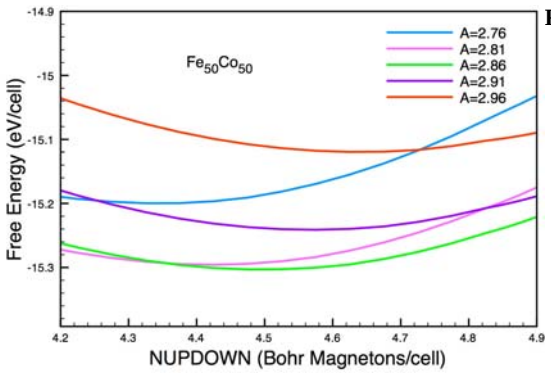


The structure of Fe16N2 is body-centered tetragonal



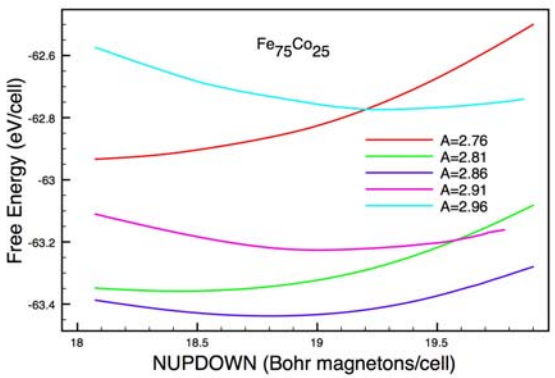
Fe Moment vs. number of Co nearest neighbors

Calculations for FeCo showed a correlation between the magnetic moment of the Fe atoms and the number of Co nearest neighbors in the cell. Here we plot the Fe moment as a function number of Co nearest neighbors



FeCo Energy vs. Moment

Sometimes VASP will converge to a local energy minimum rather than the true ground state. To be sure of finding the true ground state, we calculated the energy as a function of the total magnetic moment for different lattice constants. These calculations were for a two atom cell.

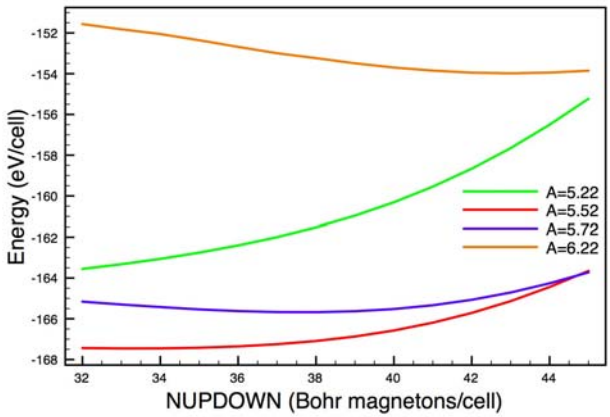


FeCo Energy vs. Moment

Energy is plotted as a function of magnetic moment per cell for eight atom cell with 6 Fe and 2 Co atoms. It can be seen that the magnetic moment increases with lattice constant.

The early reports of an ultra-high moment in $Fe_{16}N_2$ are contained in papers from Sugita and Takahashi. These results were supposedly achieved experimentally though they have not been corroborated. Here, the potential for an ultra-high moment is examined from calculations using VASP.

$Fe_{16}N_2$ Energy v. Moment



In the same manner as FeCo, after VASP converged initially to a minimum, we fixed the magnetic moment and examined the resulting change in energy. While the curve with the experimental lattice constant, 5.72 Angstroms, had its minimum at ~2.375 Bohr magnetons per Fe atom, there seems to be another possible ground state with a different lattice constant, 5.52 Angstroms and a smaller moment.

Conclusions for FeCo and $Fe_{16}N_2$

In FeCo, we found a rise in the Fe moment due to the Co nearest neighbors. Cells constructed to take advantage of this effect, however, did not yield moments exceeding the peak in the Slate-Pauling curve. For $Fe_{16}N_2$, we did not find any support for the reports of ultra-high moments around 3.5 Bohr magnetons per Fe atom. Our results indicate the ground state occurs with a different lattice constant than experimentally reported, and this lattice constant of 5.52 Angstroms has a relatively low moment.

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