Search for High Magnetization (FeCo and Fe\textsubscript{16}N\textsubscript{2})

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FeCo and Fe\textsubscript{16}N\textsubscript{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\textsubscript{16}N\textsubscript{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).

FeCo

The structure of Fe\textsubscript{16}N\textsubscript{2} is body-centered tetragonal

Fe\textsubscript{16}N\textsubscript{2}

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 of the 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.

Conclusions for FeCo and Fe\textsubscript{16}N\textsubscript{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 Slater-Pauling curve. For Fe\textsubscript{16}N\textsubscript{2}, we did not find any support for the reports of ultra-high moments around 3.5 Bohr magnetons per Fe atom, but there seems to be another possible ground state with a different lattice constant, 5.52 Angstroms and a smaller moment.

Fe\textsubscript{16}N\textsubscript{2} Energy vs. Moment

The early reports of an ultra-high moment in Fe\textsubscript{16}N\textsubscript{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.

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