Exchange Interactions in CrO$_2$

H. Sims, W. H. Butler  
Center for Materials for Information Technology  
The University of Alabama  
James M. MacLaren  
Tulane University, New Orleans, LA 70118

This project was funded by NSF grants DMR-0213985 and DMR-0706280 and by Graduate Fellowships from the University of Alabama.

CrO$_2$ is of great fundamental interest because it is one of relatively few ferromagnetic oxides and the only material that has been experimentally demonstrated to be a half-metal. CrO$_2$ represents one of very few cases in which superexchange mediated by intervening oxygen atoms promotes ferromagnetic alignment rather than anti-ferromagnetic. Because CrO$_2$ is half-metallic with a relatively large gap at the Fermi energy in the minority spin channel we expect that its spin wave spectrum will not be damped by the generation of low energy electron-hole pairs. Here we report on exchange interactions in bulk CrO$_2$ calculated from first-principles. We considered three near neighbor interactions, the interaction between the corner and body center which is mediated through a single Oxygen atom, the interaction between a Cr and the Cr directly "above" it in the (001) direction also mediated by a single Oxygen atom, and the interaction between a Cr and its neighbor in the (100) direction mediated by two intervening oxygen atoms. The interactions were calculated by rotating one or more of the Cr ions while constraining the others to remain parallel. We then fitted the resulting energy vs. angle data to $1 - \cos(\theta)$ and extracted exchange energy parameters with a least-squares method.

We calculated the (100), (001), and (111) exchange coefficients using the recently-added spin spiral method in VASP. The first order $J_{100}$ ought to be identical in the (100) and (001), as each corresponds to $J_{111}$. By convention, positive coefficients indicate ferromagnetic coupling and negative coefficients indicate antiferromagnetic coupling.

We calculated the (100), (001), and (111) exchange coefficients using a standard supercell method, rotating individual moments as indicated in the table in the upper left. The dashed lines indicate the fit to $1 - \cos(\theta)$. We calculate $J_{100} = -0.0136$ eV, $J_{001} = 0.0248$ eV, and $J_{111} = 0.0250$ eV.

Conclusions and Future Work

Exchange interactions were calculated for CrO$_2$ using supercells and spin spirals. We did not obtain satisfactory agreement between the two methods, but we have reason to believe that further k-point convergence will yield good agreement. We plan to investigate exchange interactions near CrO$_2$-RuO$_2$ and CrO$_2$-SnO$_2$ interfaces.