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DFT + QMC study of Iron Oxide

Joshua Townsend & Luke Shulenburger

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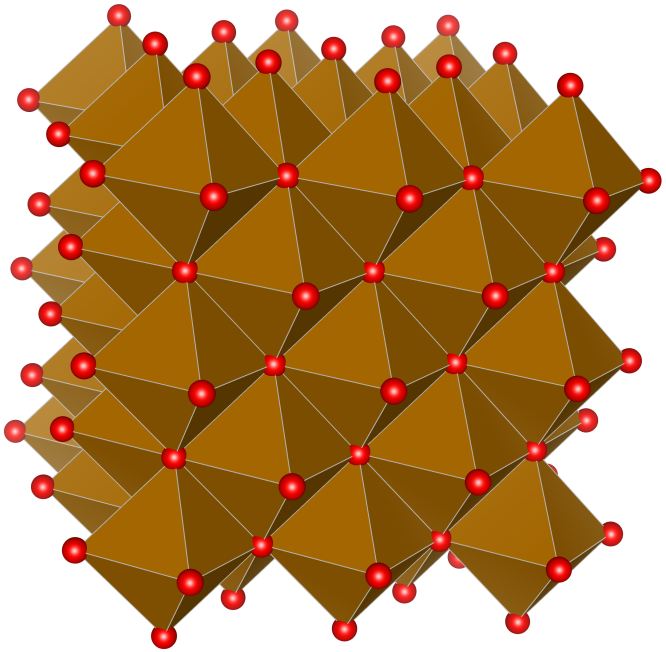
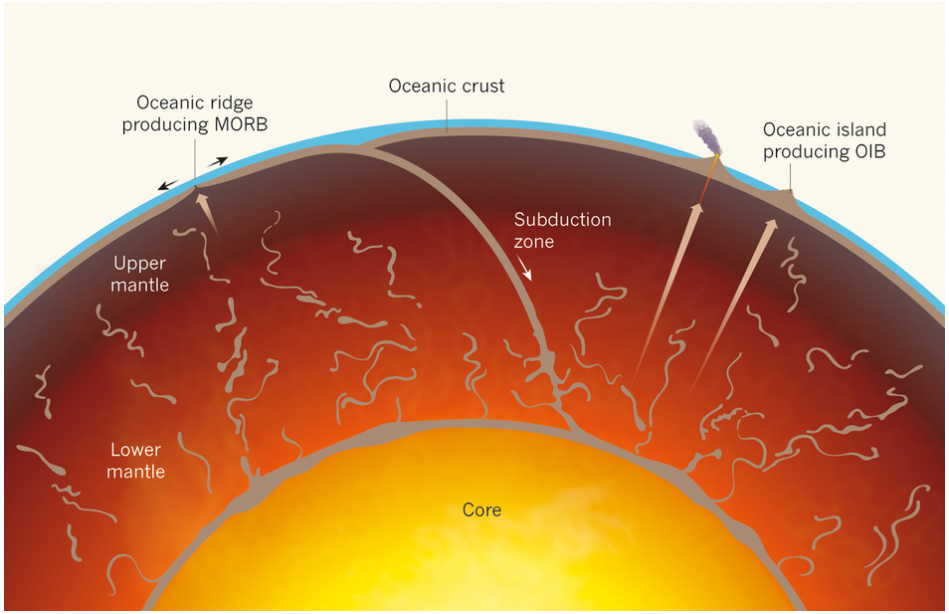
FeO :: Easy chemistry, hard physics





Woodhead 2015

- Important system in geophysics - (Mg, Fe)O abundant in Earth.

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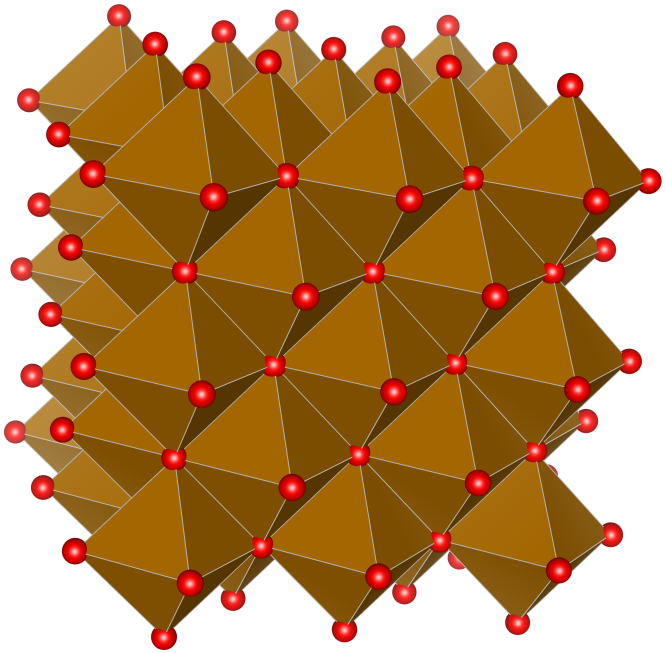

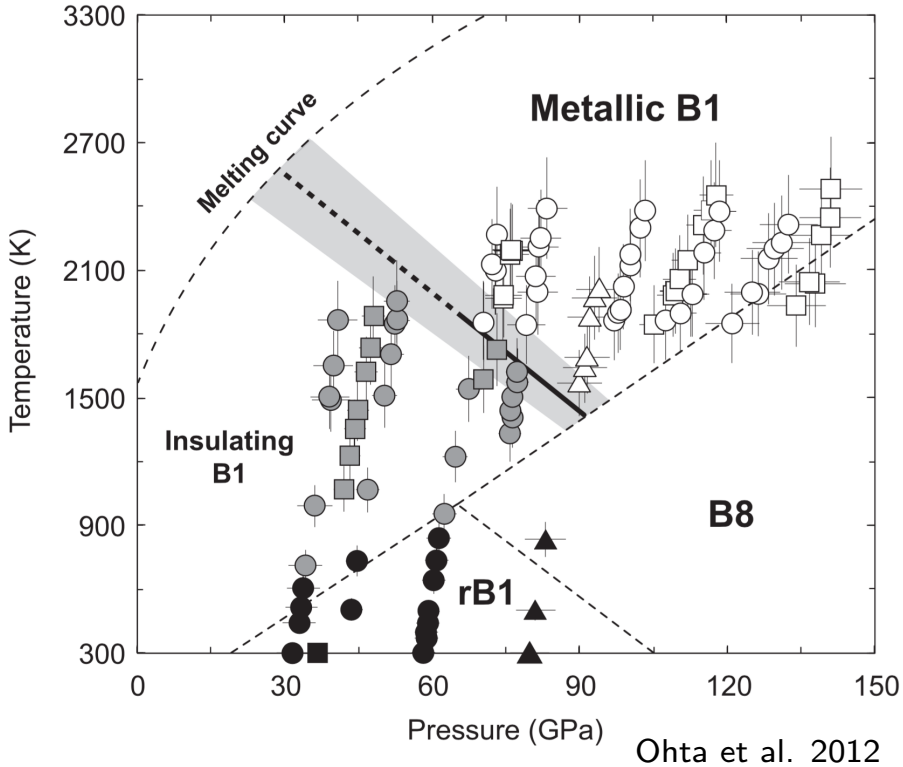

Ohta et al. 2012

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- Multiple electronic, magnetic, and structural phase transitions.

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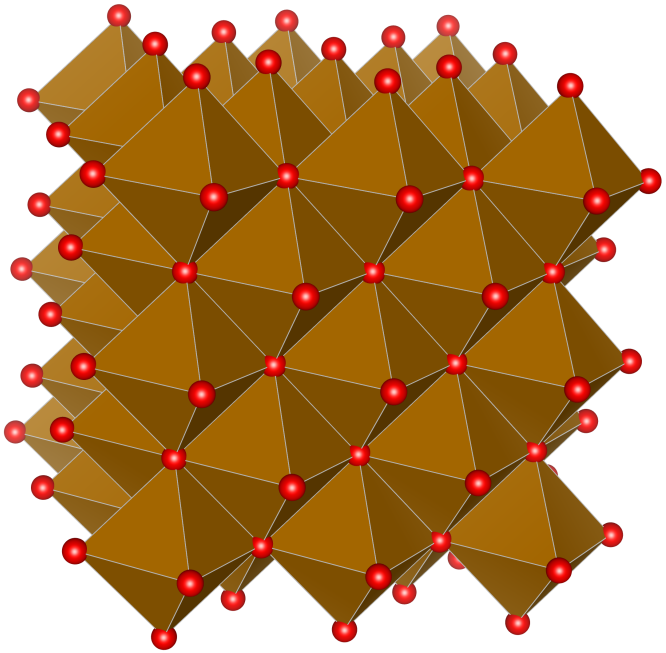
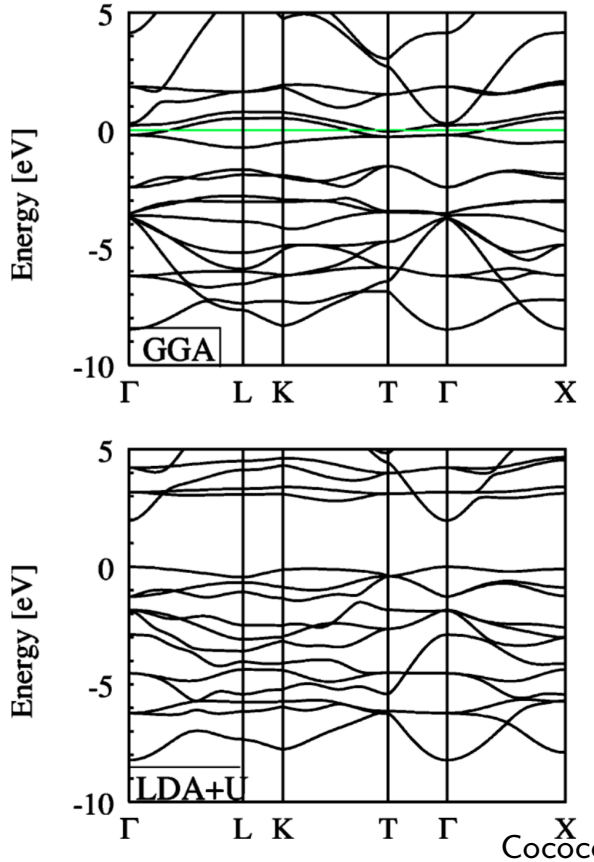
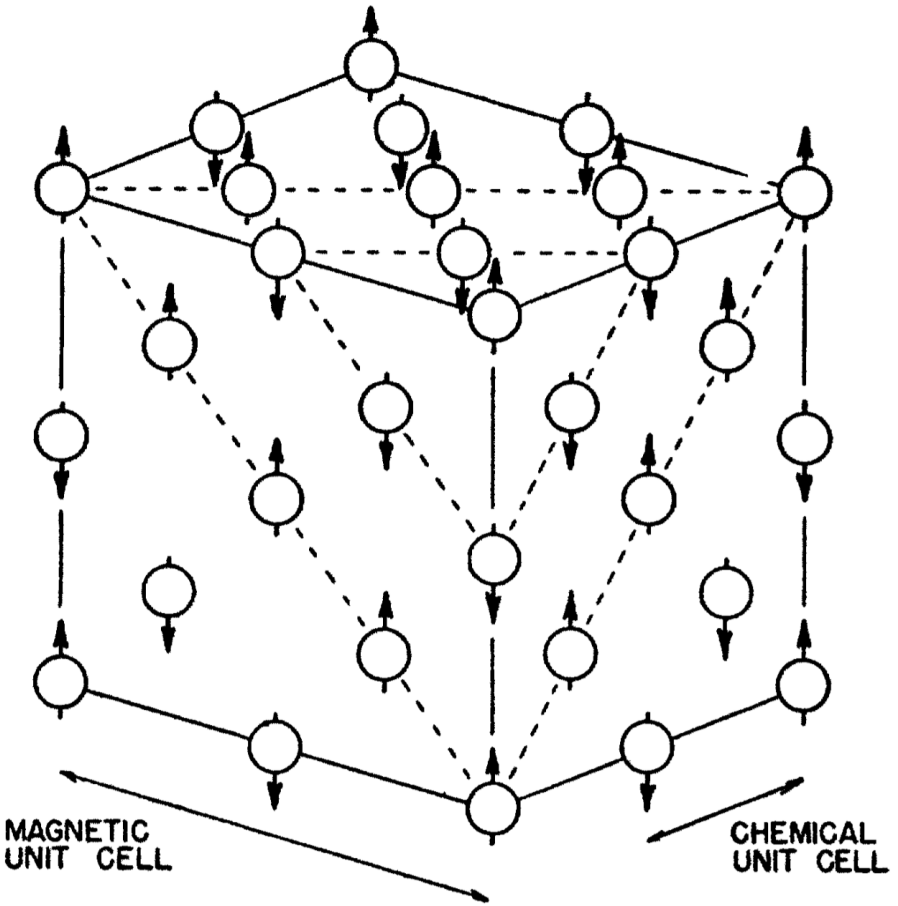




Cococcioni et al. 2005

- Important system in geophysics - (Mg, Fe)O abundant in Earth.
- Multiple electronic, magnetic, and structural phase transitions.
- Vanilla DFT fails to reproduce B1 insulating state - Mott insulator.

Magnetoelastic coupling in FeO at low temperature



Shull et al. 1951

$T < 198$ K - FM ordering on [111]

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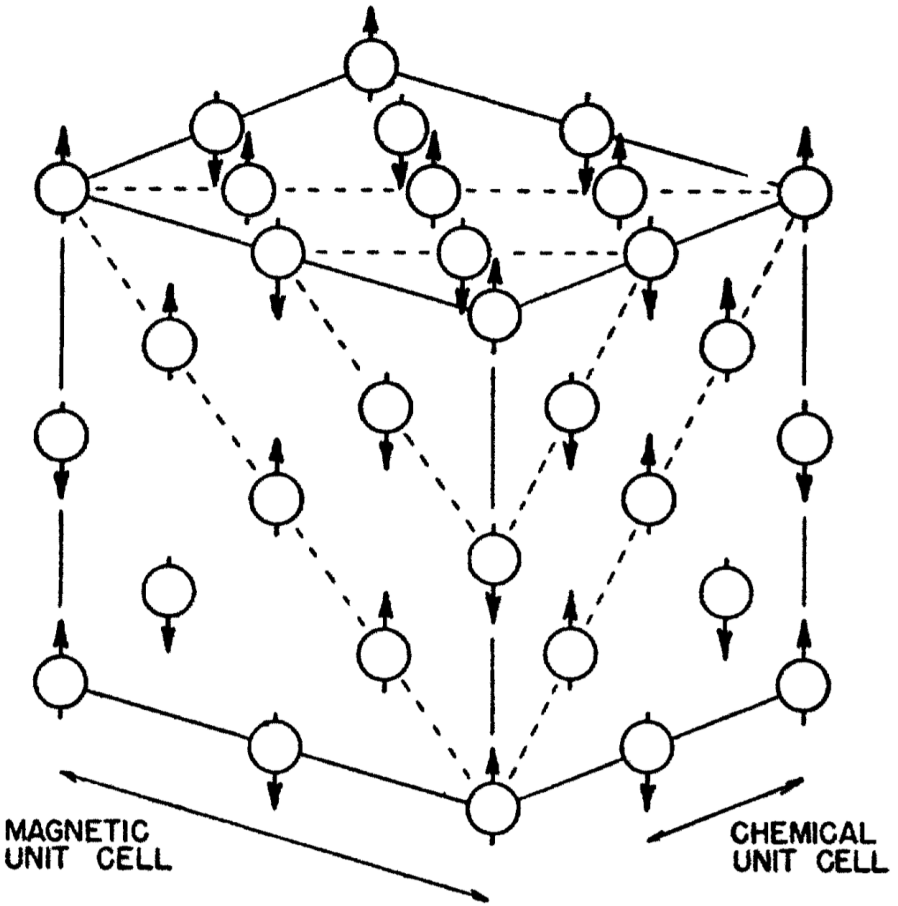

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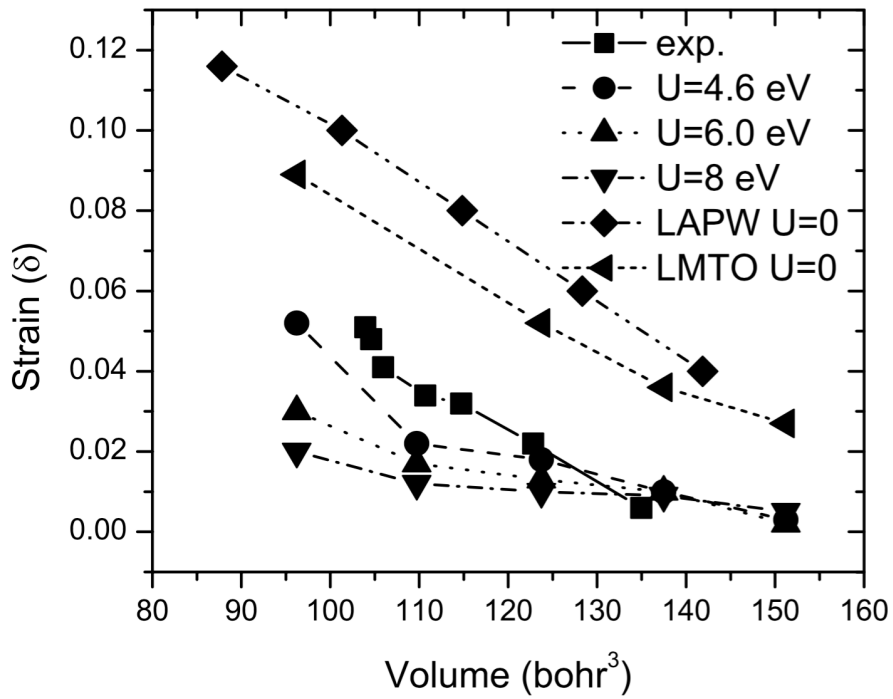
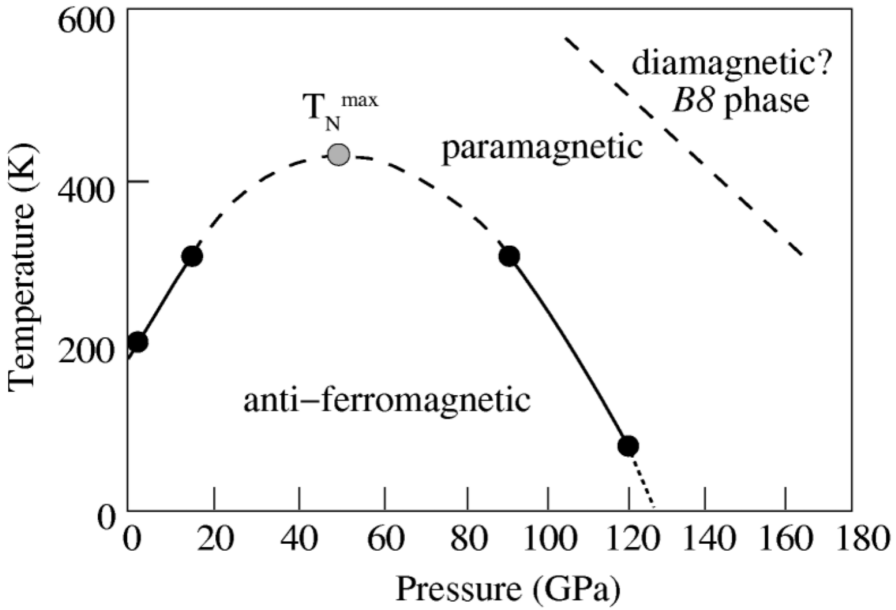


Gramsch et al. 2003

$T < 198$ K - FM ordering on [111]

Induced rhombohedral strain due to AFM structure.

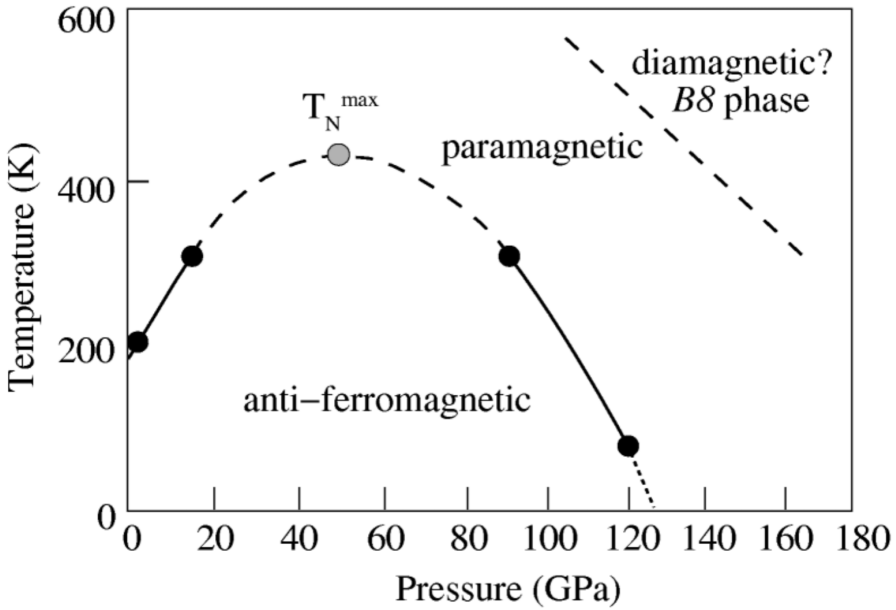
Magnetic moment collapse & MIT at low temperature



Badro et al. 1999

Experiments suggest magnetic collapse at high pressure - but can't distinguish PM or DM

Magnetic moment collapse & MIT at low temperature



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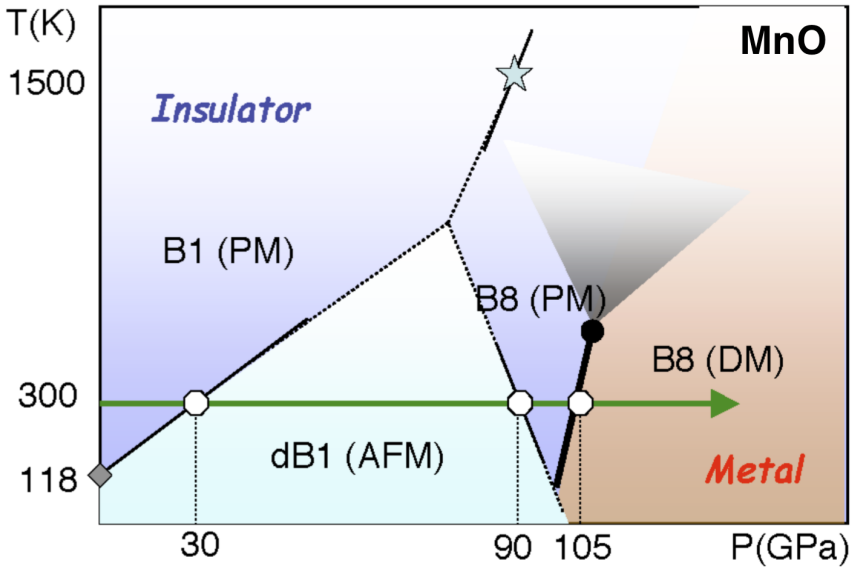

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Observed in MnO at low T @ $P \approx 1$ Mbar & accompanied by MIT

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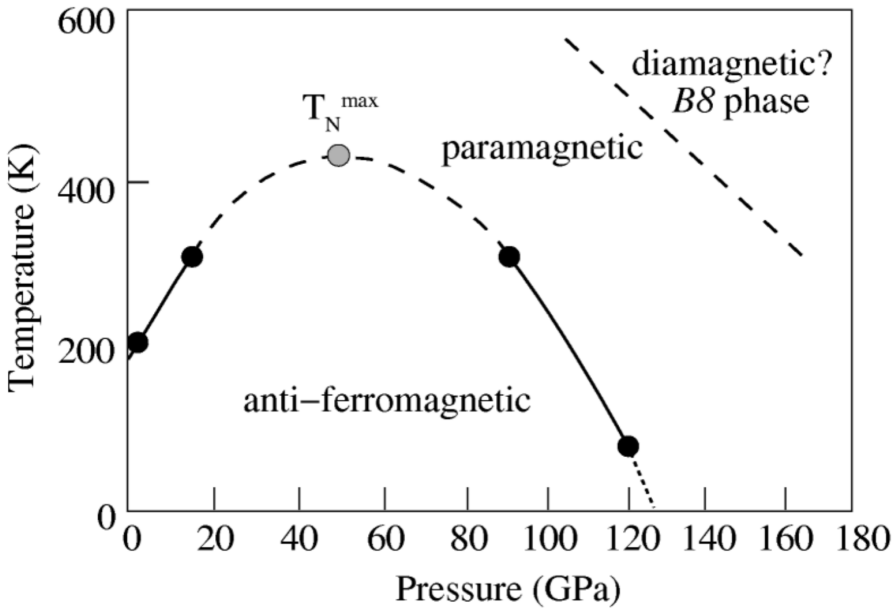

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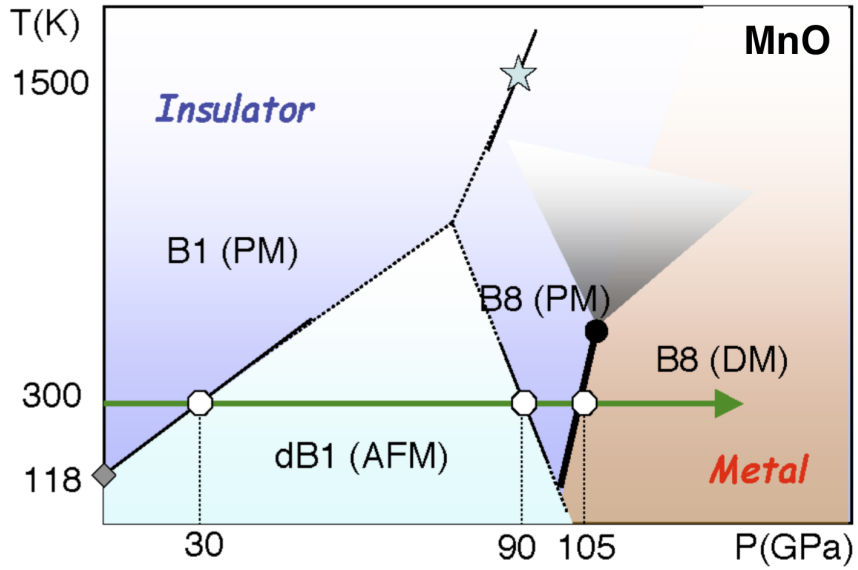

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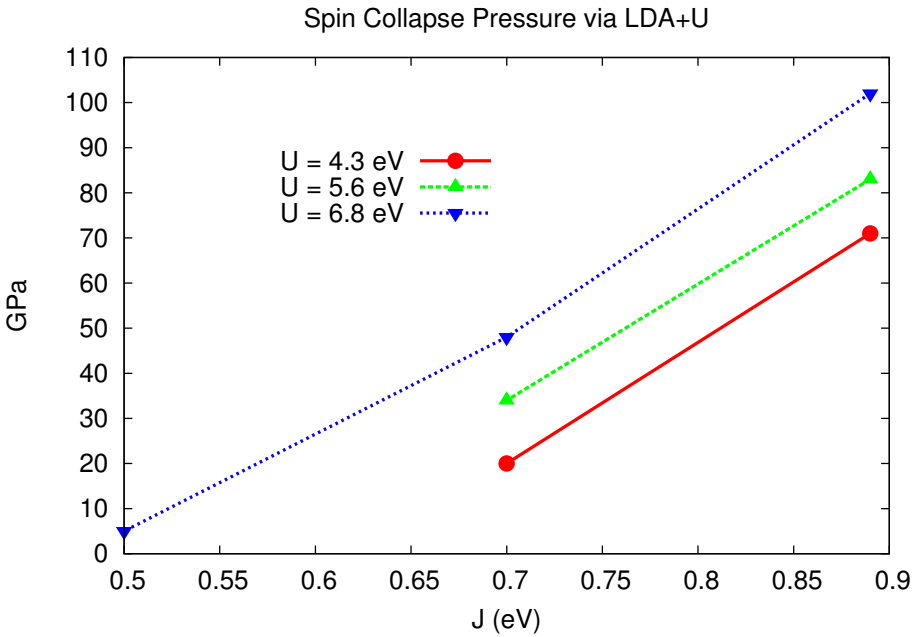
How to do a better job of predicting all these phenomena?

How to generate good trial wave functions?



B1 AFM vs B1 NM

- Magnetic collapse sensitive to J

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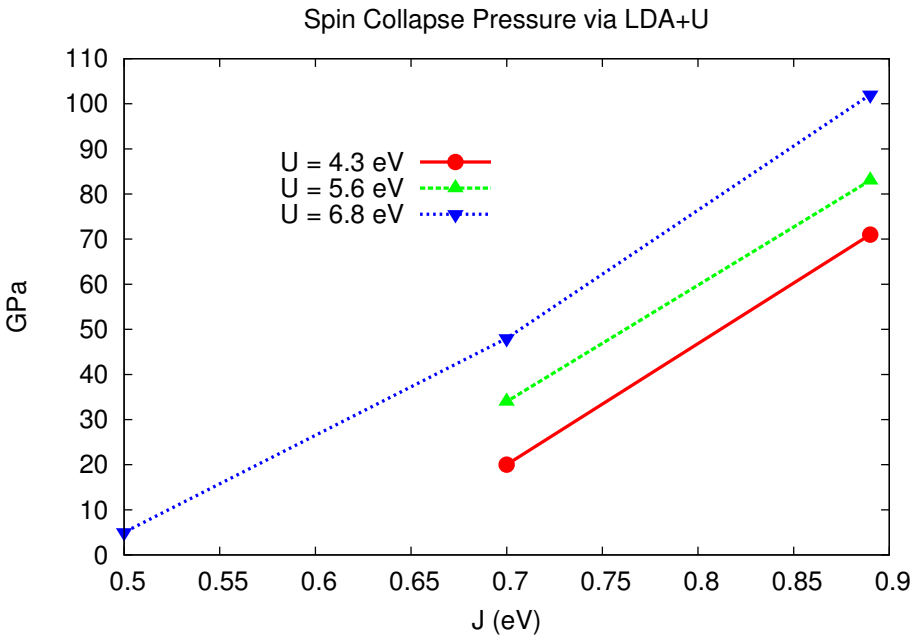

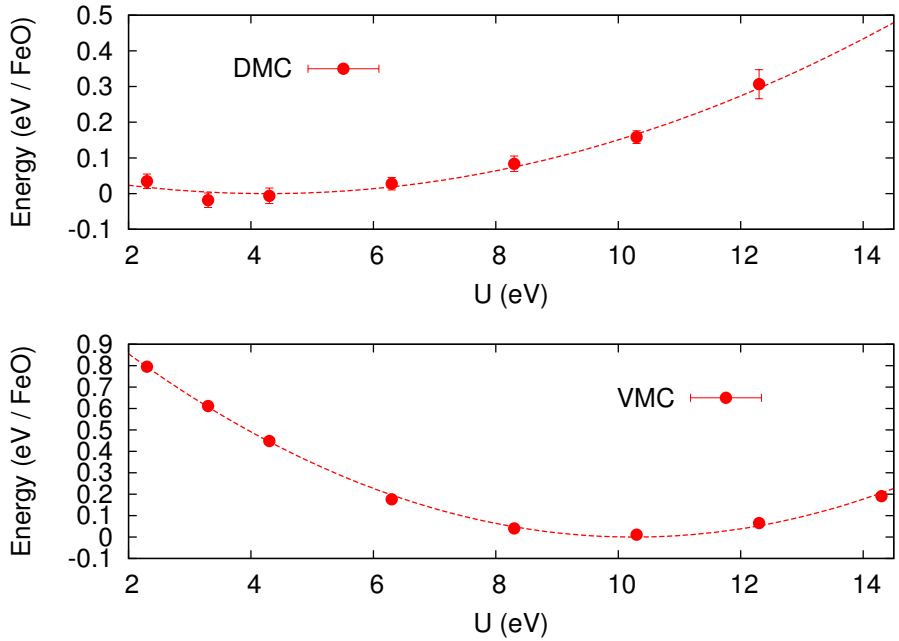

B1 AFM vs B1 NM

All points at ambient volume.

- Magnetic collapse sensitive to J
- DMC and VMC don't agree on "optimized" U

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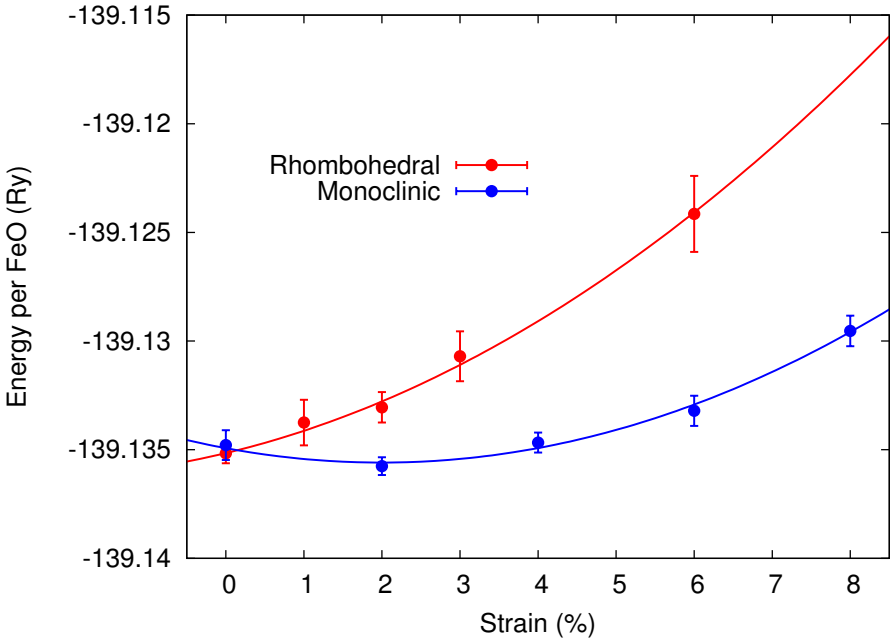

- Equilibrium strain is sensitive to *d*-matrix symmetry.

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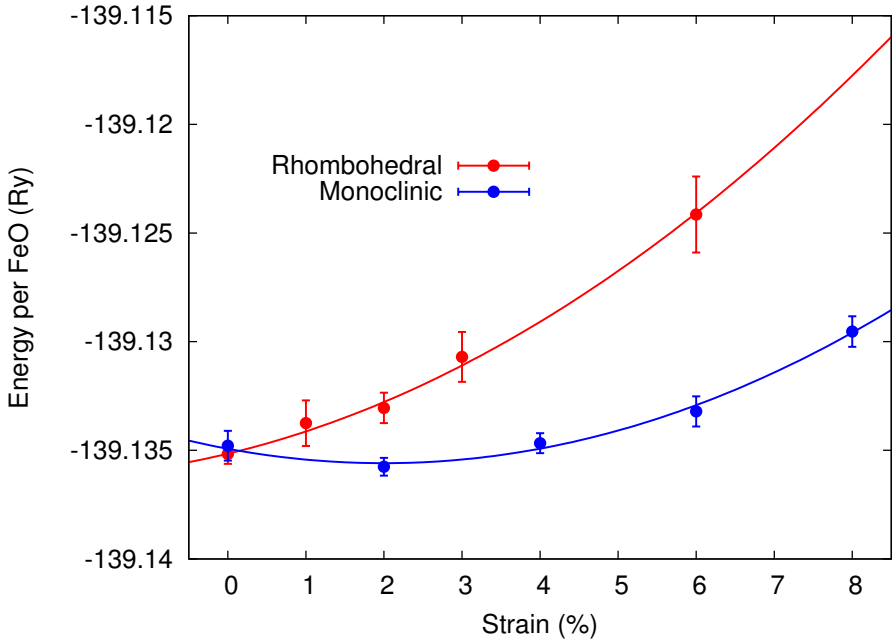
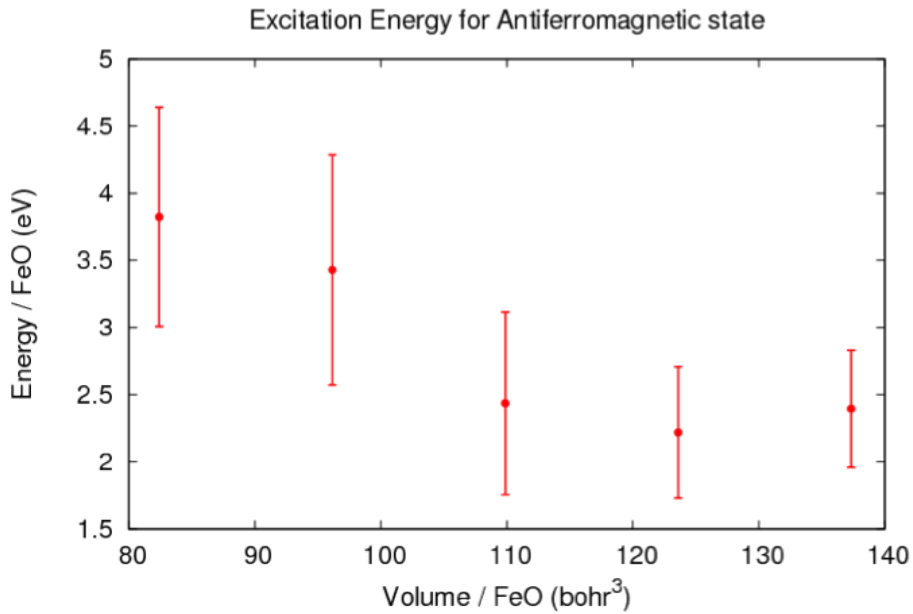
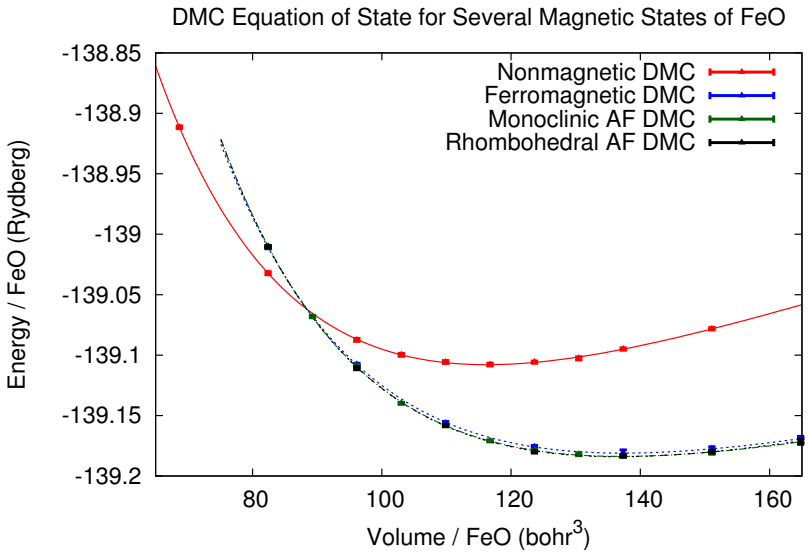




- Equilibrium strain is sensitive to d-matrix symmetry.
- No MIT transition in B1 FeO for $P < 185$ GPa

Comparing equations of state



EOS Parameter Comparison*:

Study	K_0 [GPa]	K_0' -	a_0 [Å]
Unstrained QMC	179(11)	4.8(5)	4.342(10)
Strained QMC	165(6)	4.7(3)	4.343(8)
Kolorenc QMC[1]	170(10)	5.3(7)	4.324(6)
Isaak LDA[2]	173	4.2	4.136
Fisher expt.[3]	149(1)	3.60(4)	4.334
McCammon expt.[4]	152	4.92	4.334

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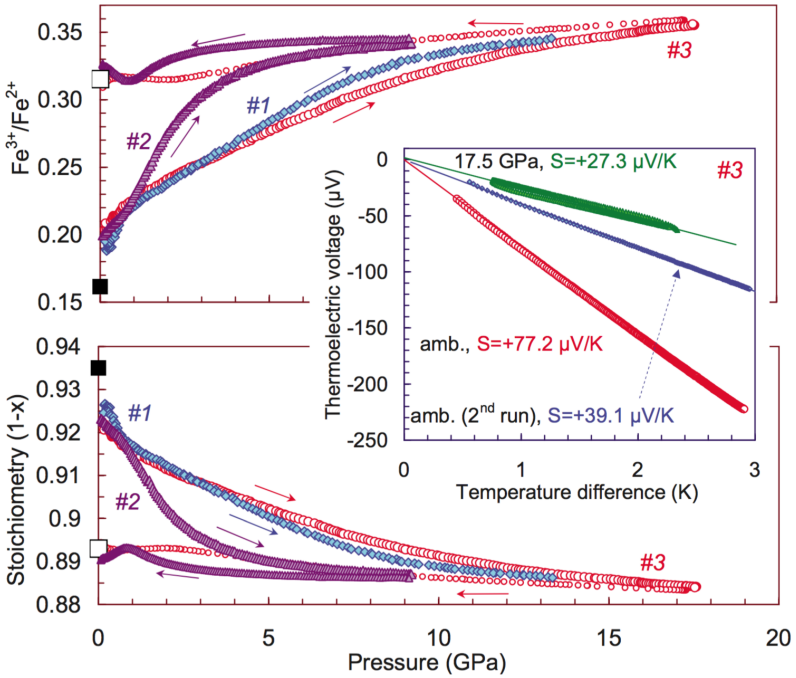

Ovsyannikov et al. 2010

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*Comparing EOS parameters is tricky! Experiments are non-stoichiometric, and everyone uses a different functional form. Additionally, there is some evidence that wüstite becomes more nonstoichiometric under pressure!

Future Work

Ongoing Research Questions:

- How to improve DFT wave functions for QMC?

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  1. New collaboration with Y Fei @ CIW - nearly stooichiometric FeO