LDA+U Picture of the Moment Collapse under Pressure in MnO

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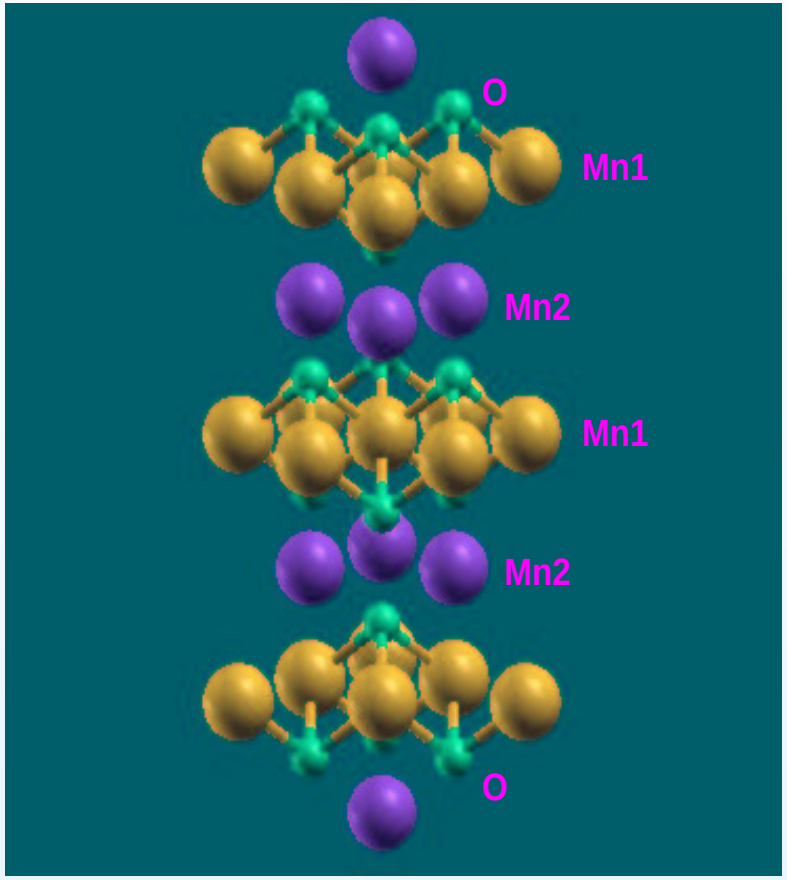
Structural Details & Calculational Methods



B1 structure with Mn moments aligned ferro−magnetically in the [111] plane, with adjacent sheets having antiparallel spin

T_N = 118 K

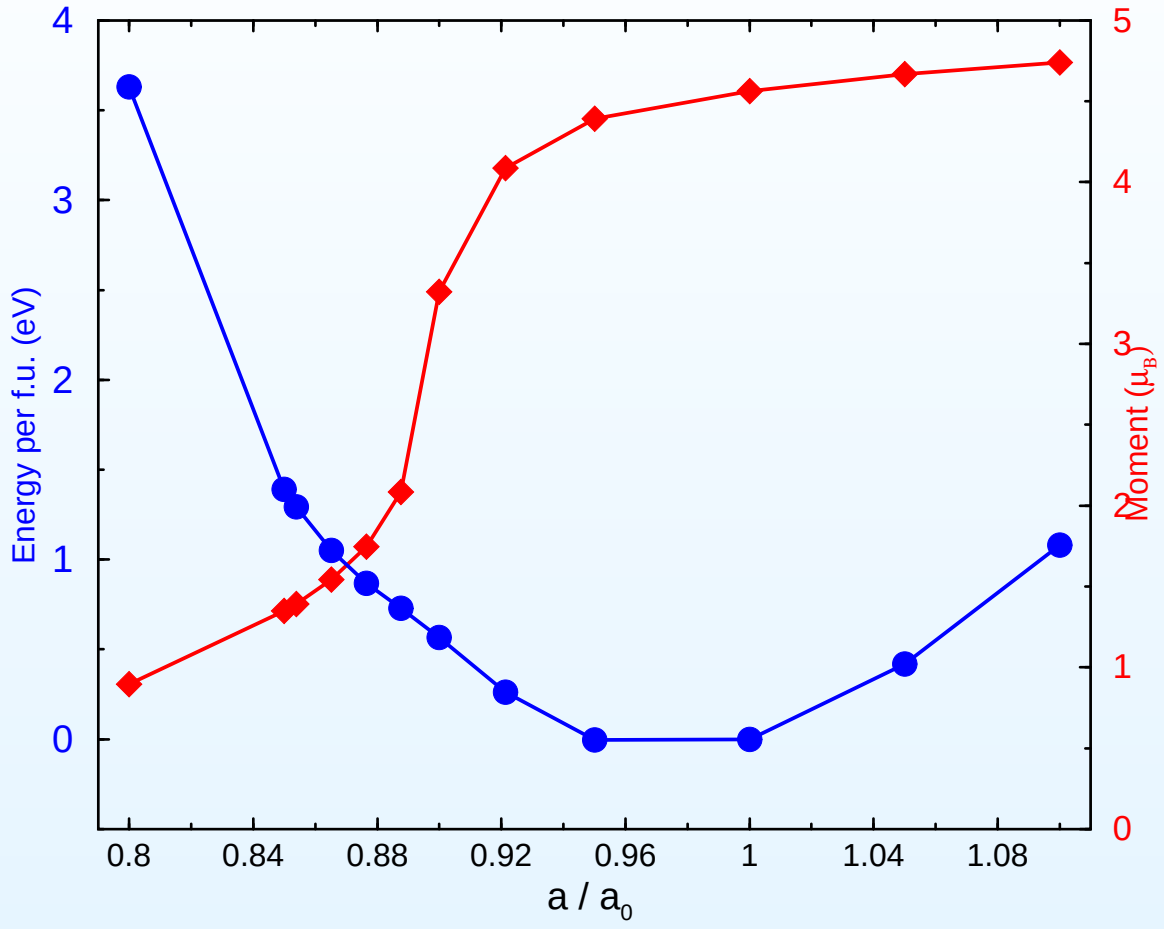
Bulk Modulus = 170 GPa

Band Gap = 3.6 − 3.8eV

Equilibrium lattice constant = 4.45 ang

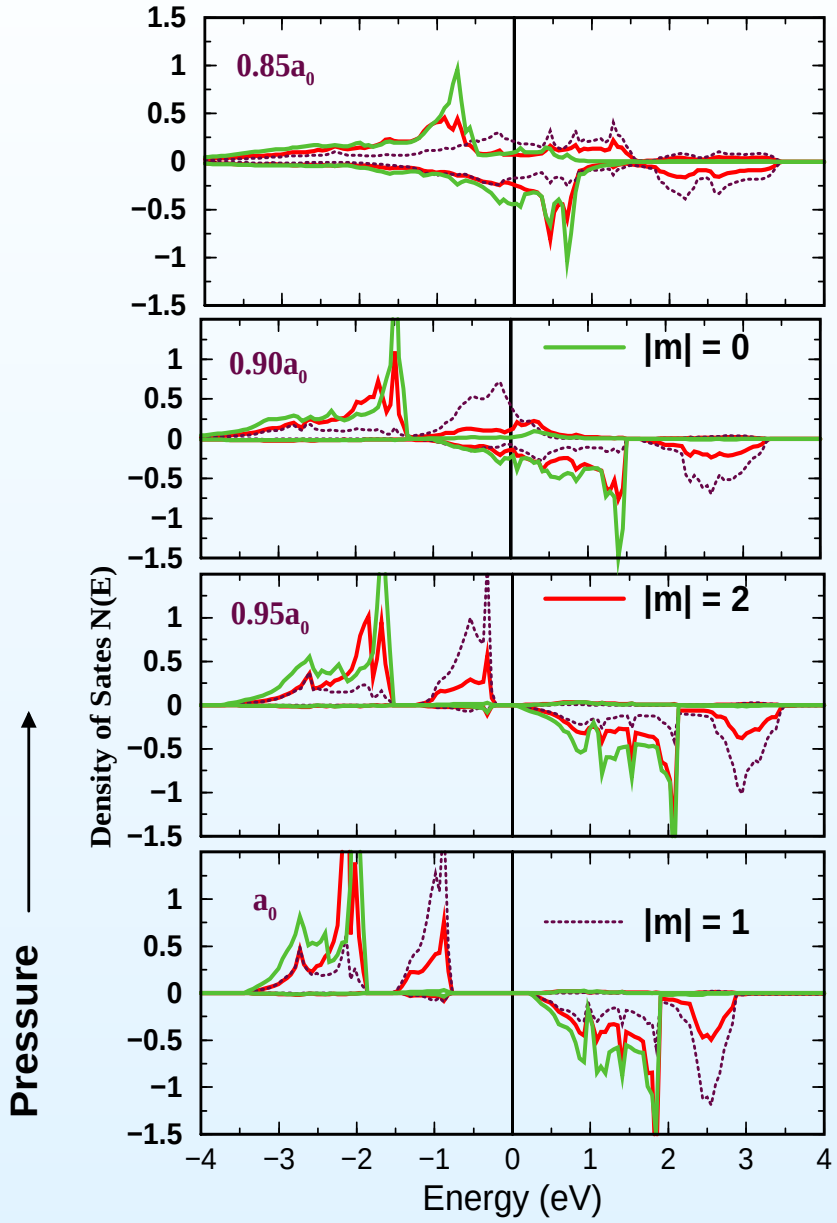
- Full Potential nonorthogonal Local-Orbital minimum-basis scheme (FPLO)

LDA : Total Energy & Moment



- Moment decreases in a continous manner with pressure
- $0.875a_o$ to $0.925a_o \rightarrow$ extremely sensitive

Density of States



In the crystal Mn atoms are in 2+ state (S = 5/2, L = 0)

All 5d orbitals are singly filled

Cubic symmetry ---> t_{2g}, e_g

Rhombohedral sym. -- e_g, $e_{g'}$, a_g

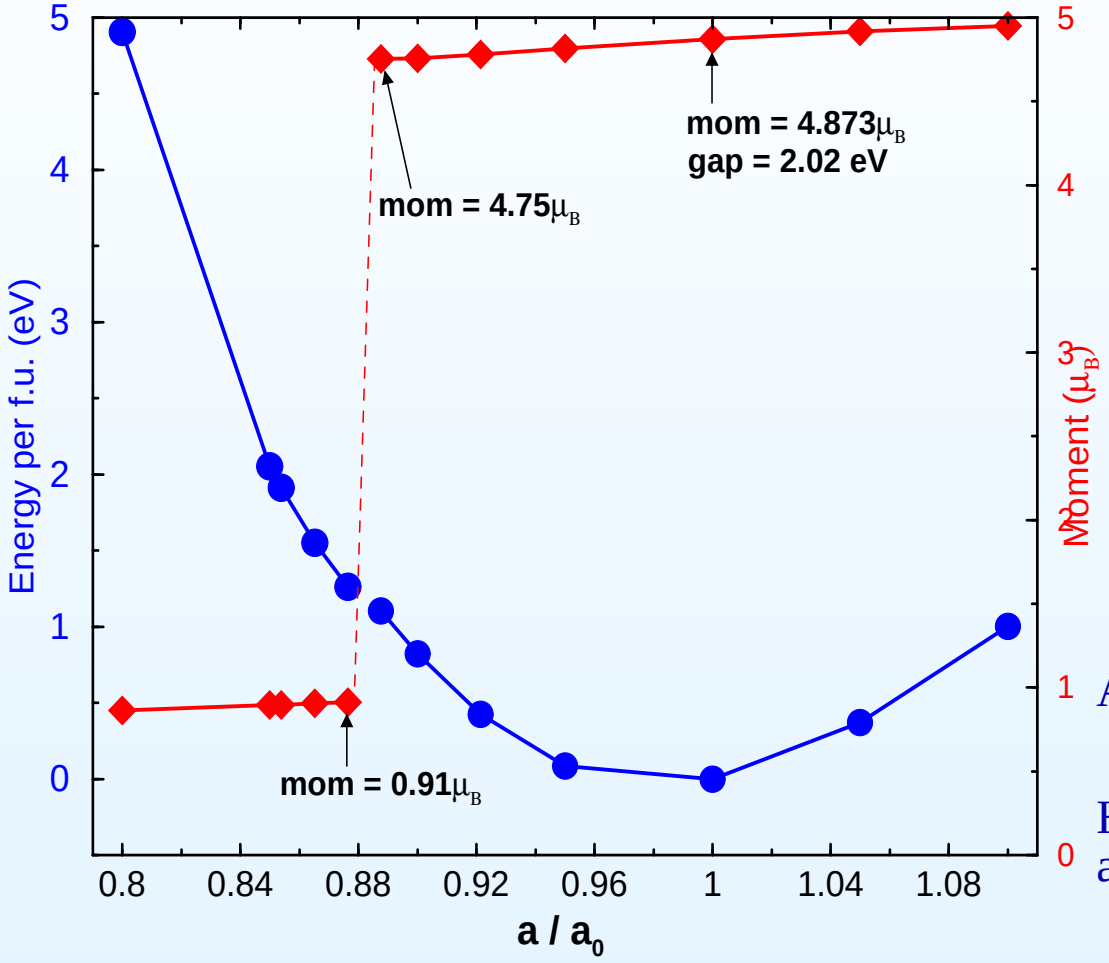
At a_0, Band Gap = 1 eV

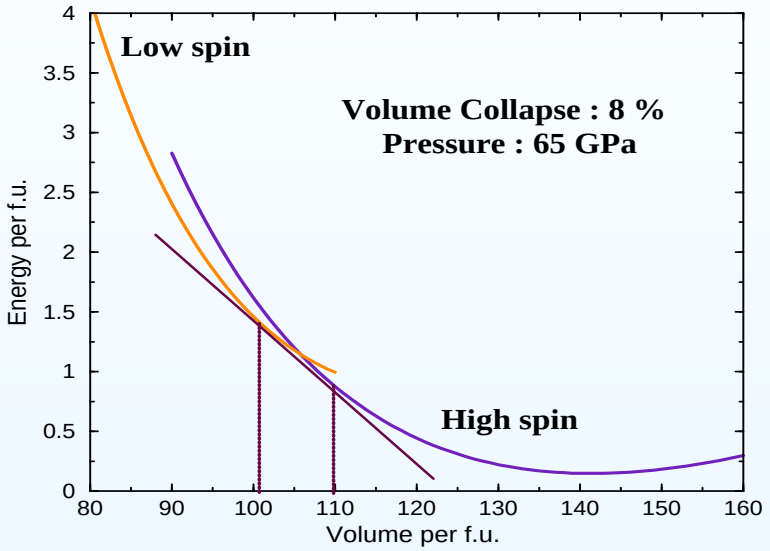
Mn d spin up states − fully occupied at equilibrium

Under pressure, bands broaden and mix spin up and down states.

Moment decreases from 4.8 to 0.8 bohr mag.

LDA+U : Total Energy & Moment (U = 5.5eV)



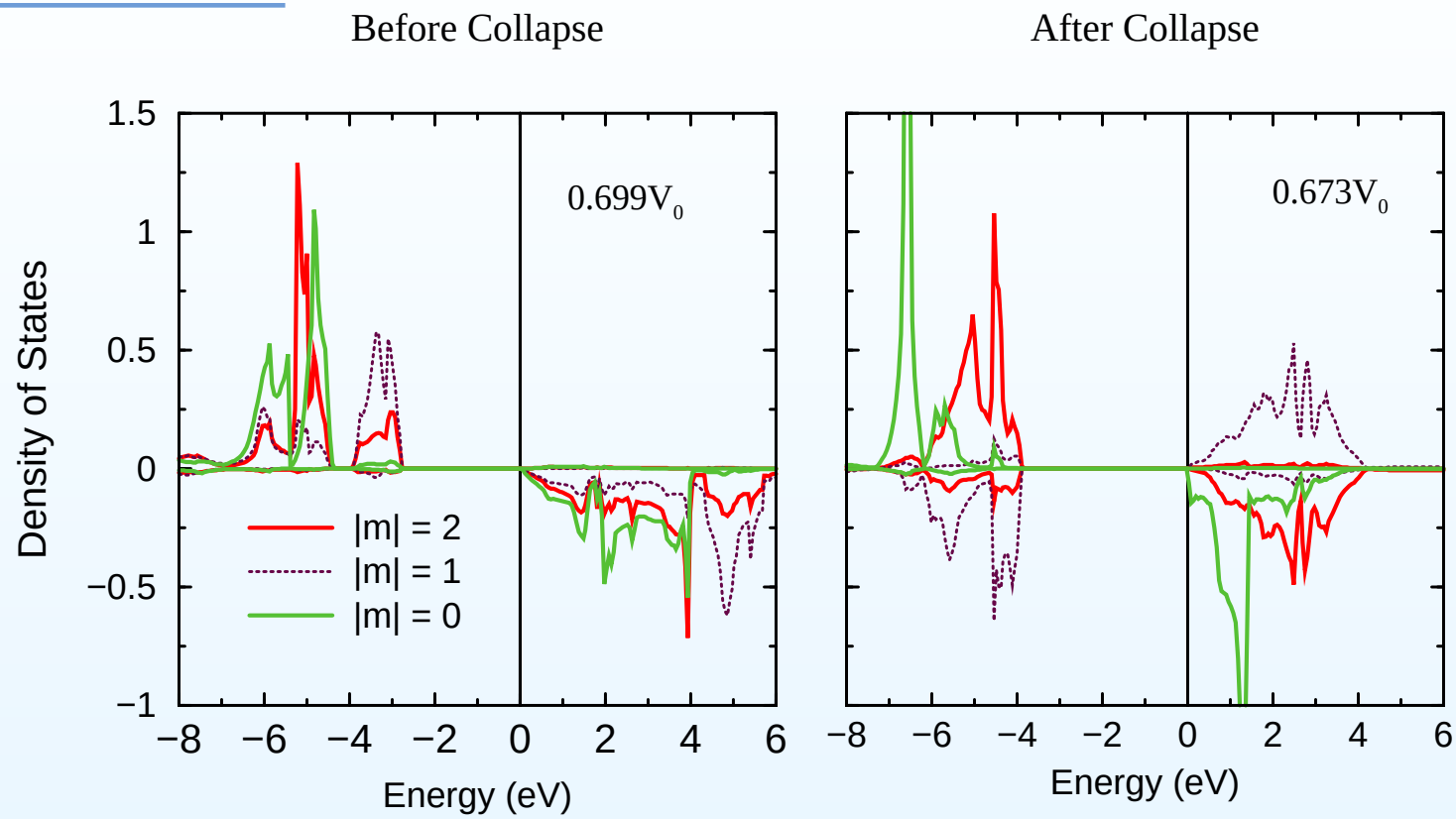


At $0.89a_0$-- First order magnetic transition

High spin to Low spin transition at 65 GPa along with a volume collapse of 7.76%

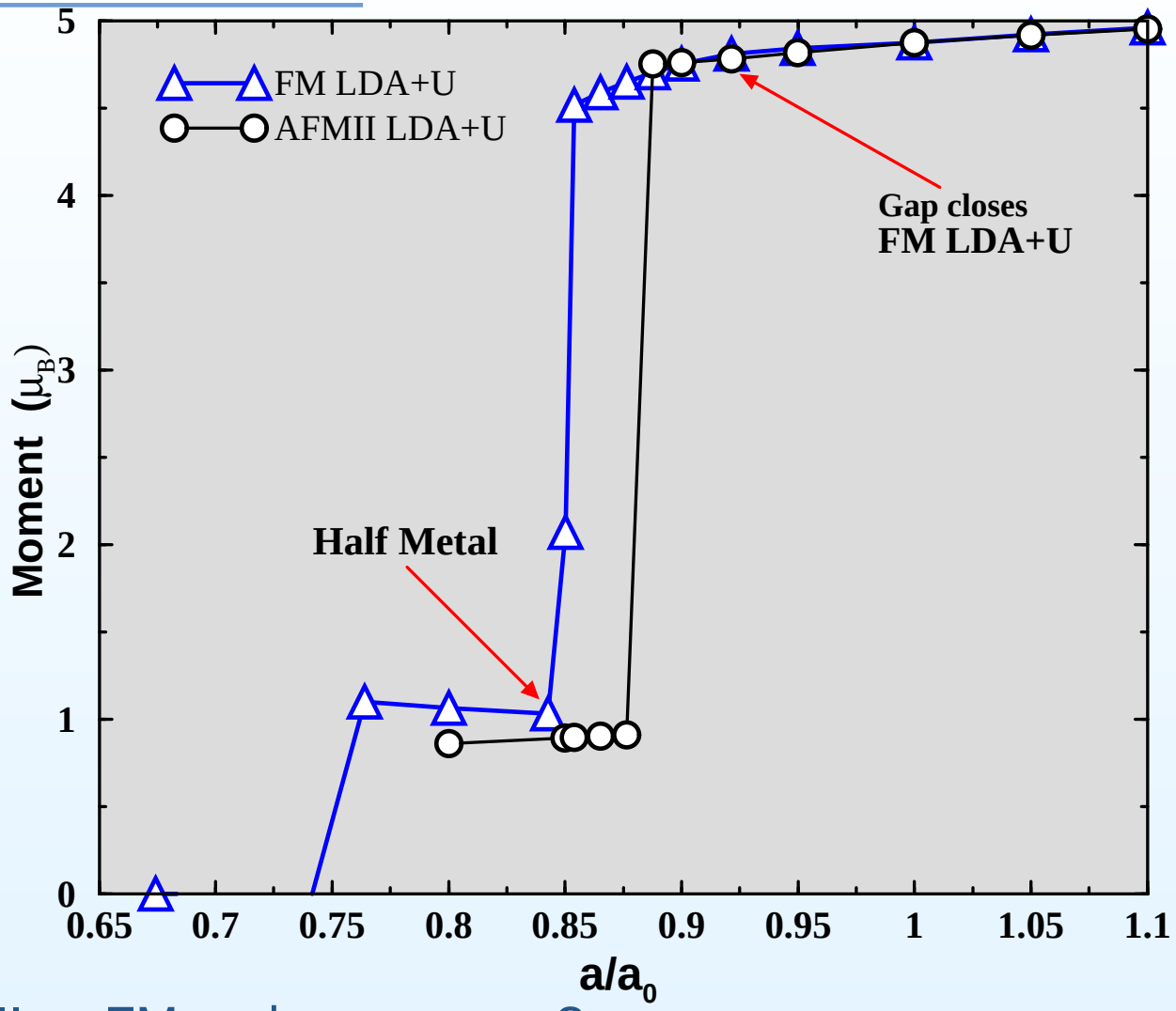
- Expt. $\rightarrow$ At 100-110 GPa, a $\approx$ 6.6% volume collapse with significant loss of moment (C.S.Yoo *etal*., PRL 2005)

Density of States



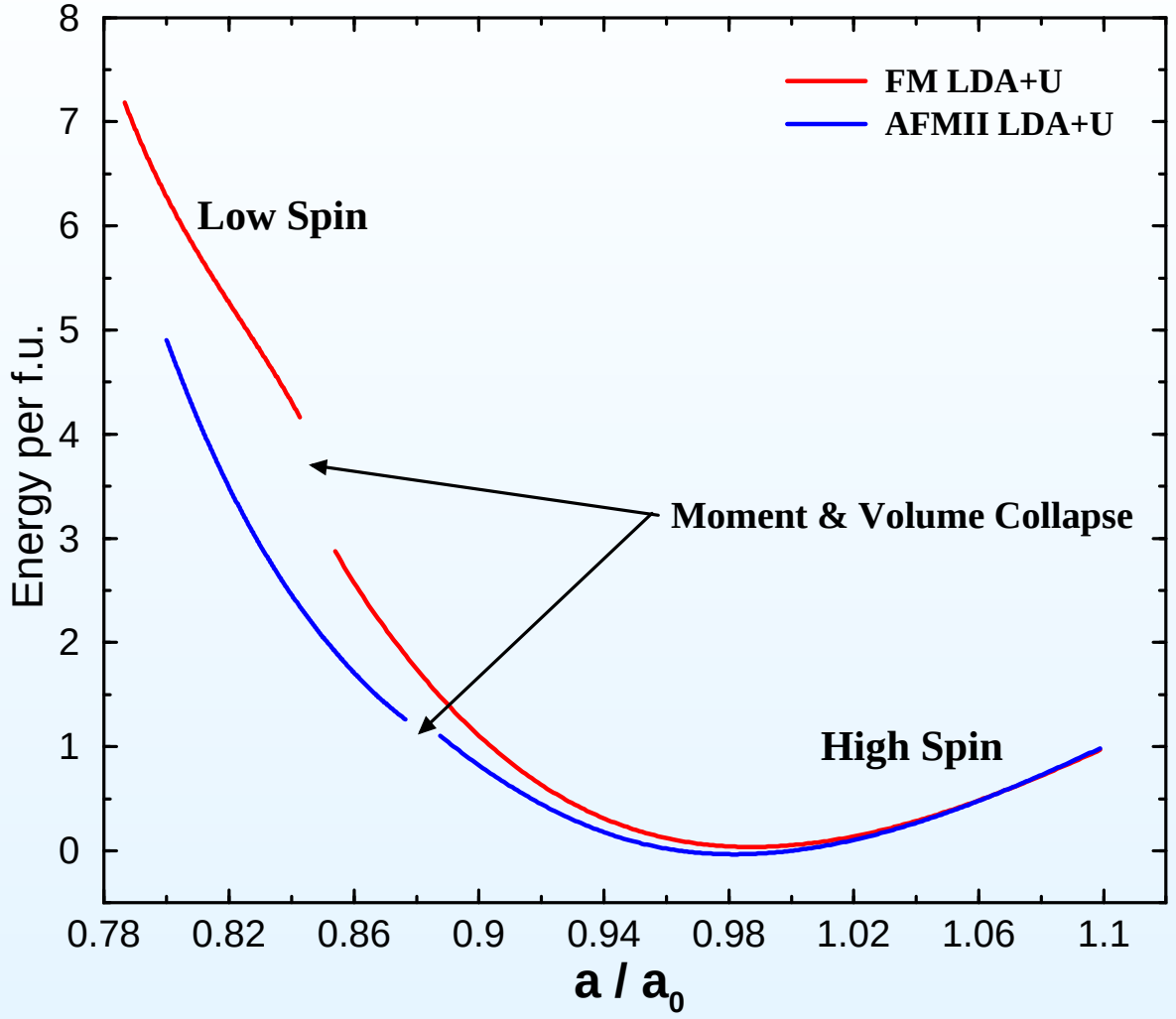
- Bandgap increases from 2.7 eV to 3.8 eV
- Before Collapse : 5 d orbitals singly occupied; spin moment $\approx 5\mu_B$
- After Collapse : Two e^- from m = $\pm$1 doublet flip; spin moment $\approx 1\mu_B$
- Both cases, total L = 0

FM & AFMII comparison



- AFMII $\rightarrow$ FM under pressure ?
- Does moment collapse happen before or after transition in magnetic order ?

FM & AFMII LDA+U comparison



- Mom. & volume collapse : AFMII - $0.69V_0$; FM - $0.61V_0$
- No AFMII $\rightarrow$ FM transition in LDA+U

Conclusions : LDA+U

- First Order magnetic transition at 65 GPa ($0.61V_0$) along with a volume collapse of 8% (AFMII)
- High spin to low spin transition governed by Oxygen coordination
- FM - Also shows moment & volume collapse at $0.69V_0$
- No AFMII $\rightarrow$ FM transition
- Exptl reports: Isostructural, first order insulator - metal transition at 100 - 110 GPa range. (C.S. Yoo et al. PRL 2005; Patterson et al., PR B 69, 220101 (2004))