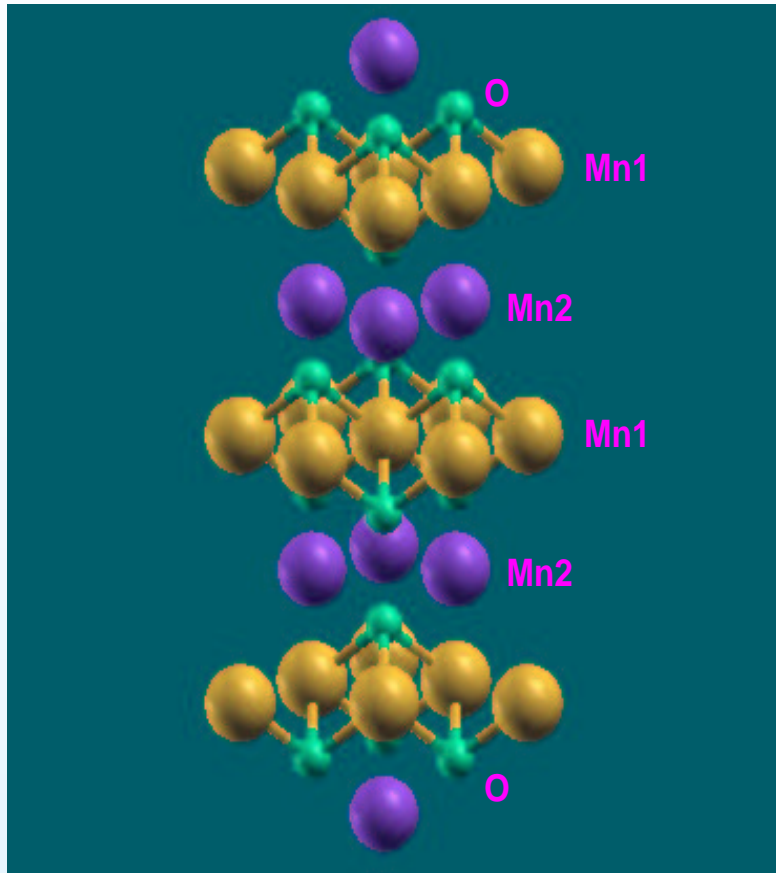


# *LDA+U Picture of the Moment Collapse under Pressure in MnO*

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# Structural Details & Computational Methods



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

$$T_N = 118 \text{ K}$$

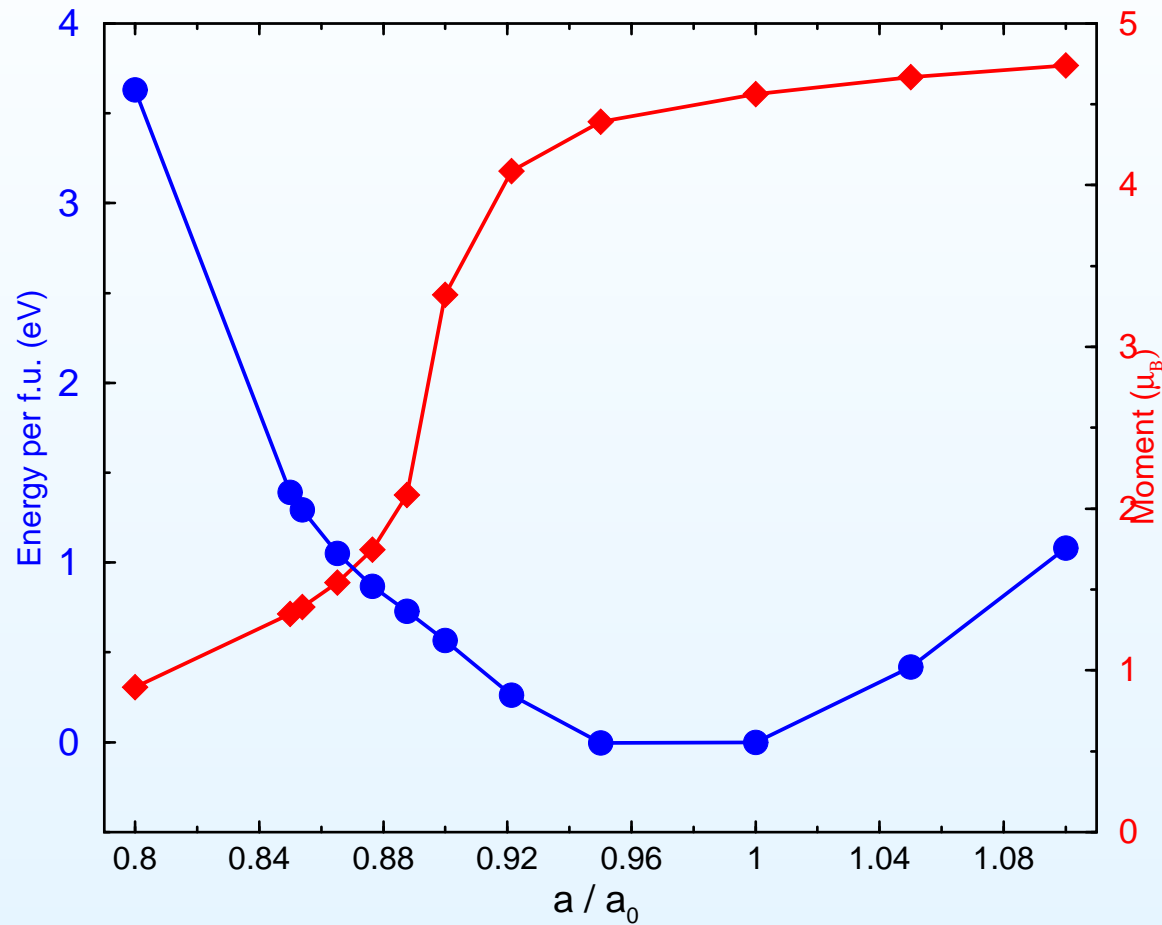
Bulk Modulus = 170 GPa

Band Gap = 3.6 – 3.8 eV

Equilibrium lattice constant = 4.45 ang

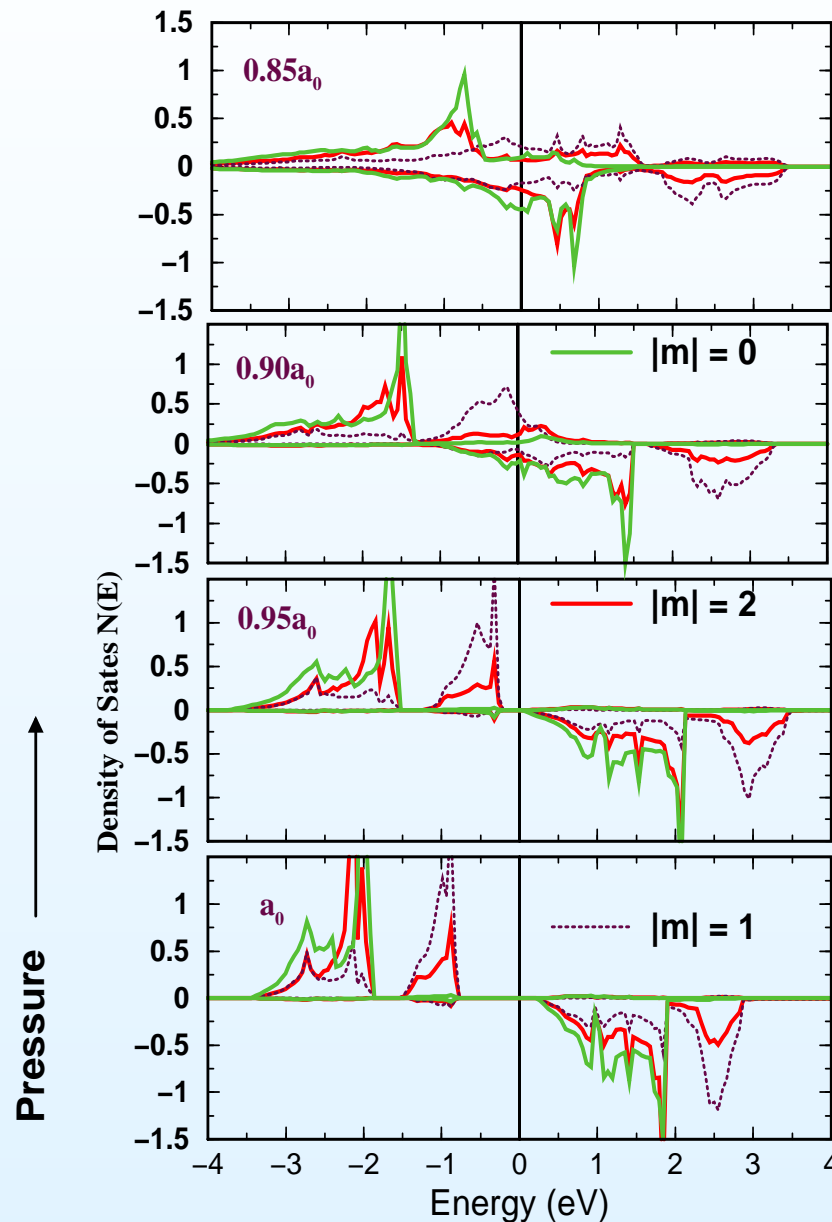
- Full Potential nonorthogonal Local-Orbital minimum-basis scheme (FPLO)

# LDA : Total Energy & Moment



- Moment decreases in a continuous manner with pressure
- $0.875a_0$  to  $0.925a_0 \rightarrow$  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  $\rightarrow t_{2g}, e_g$

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

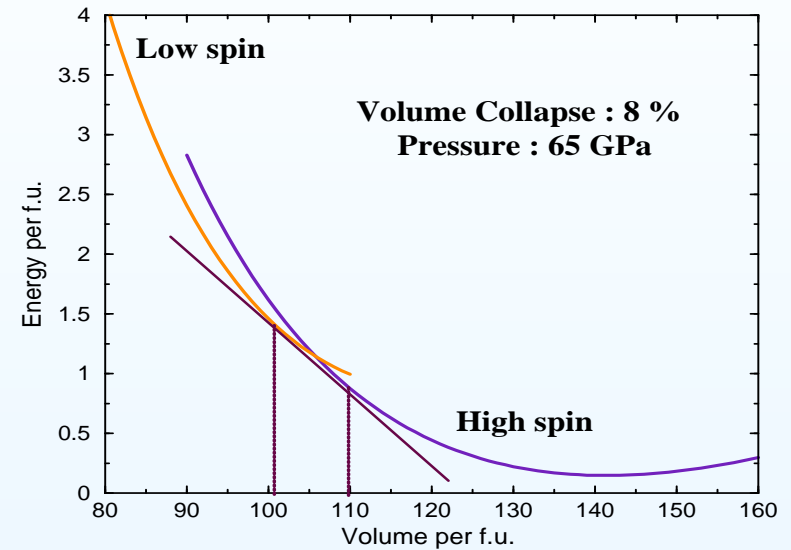
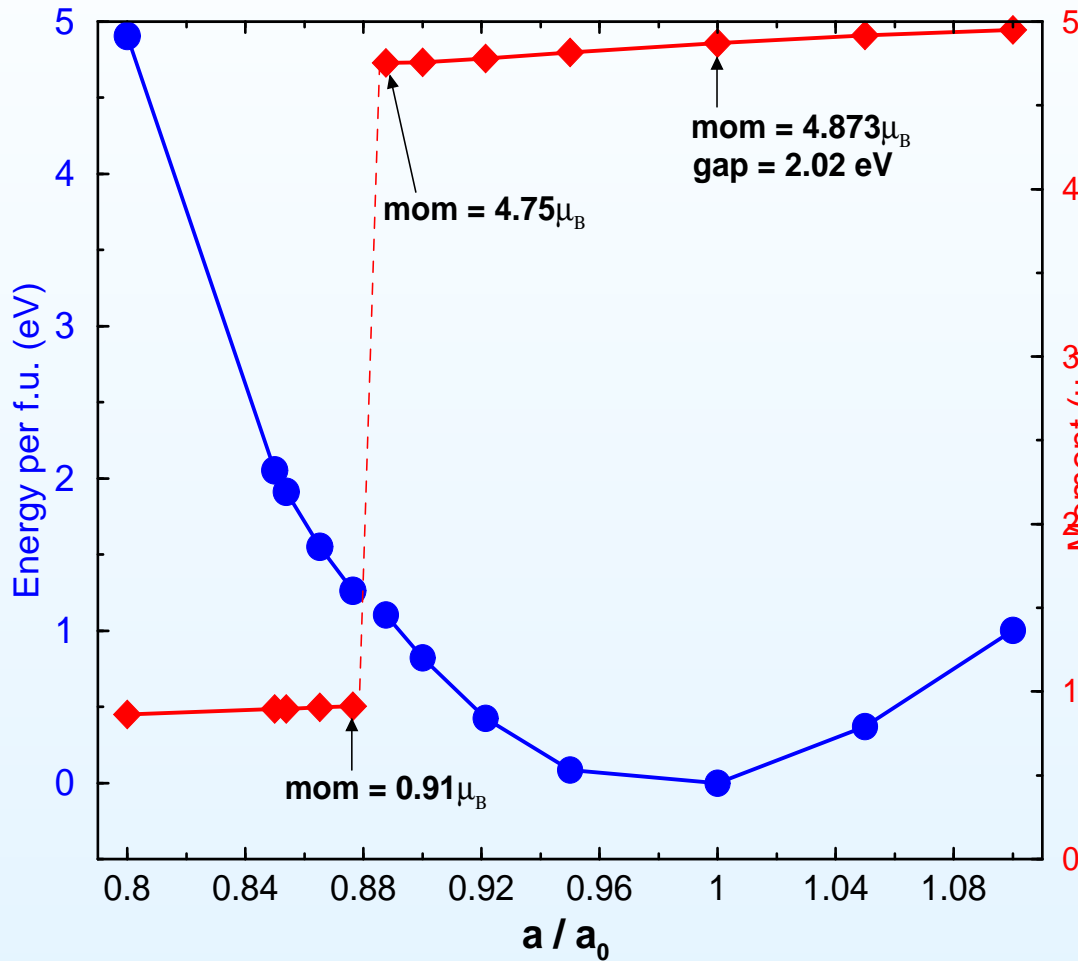
At  $a_0$ , Band Gap = 1 eV

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)

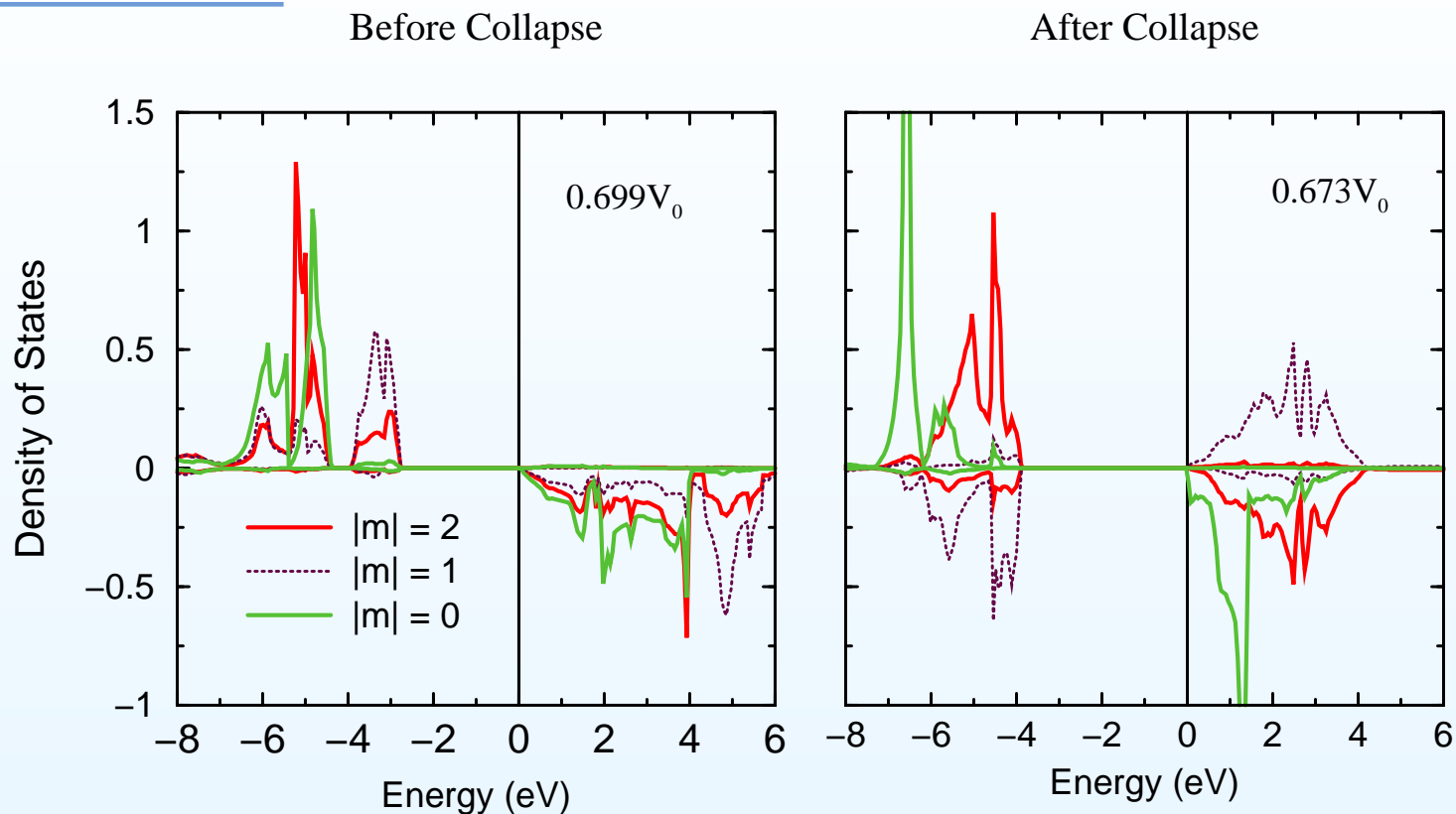


1 At  $0.89a_0$ — First order magnetic transition

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

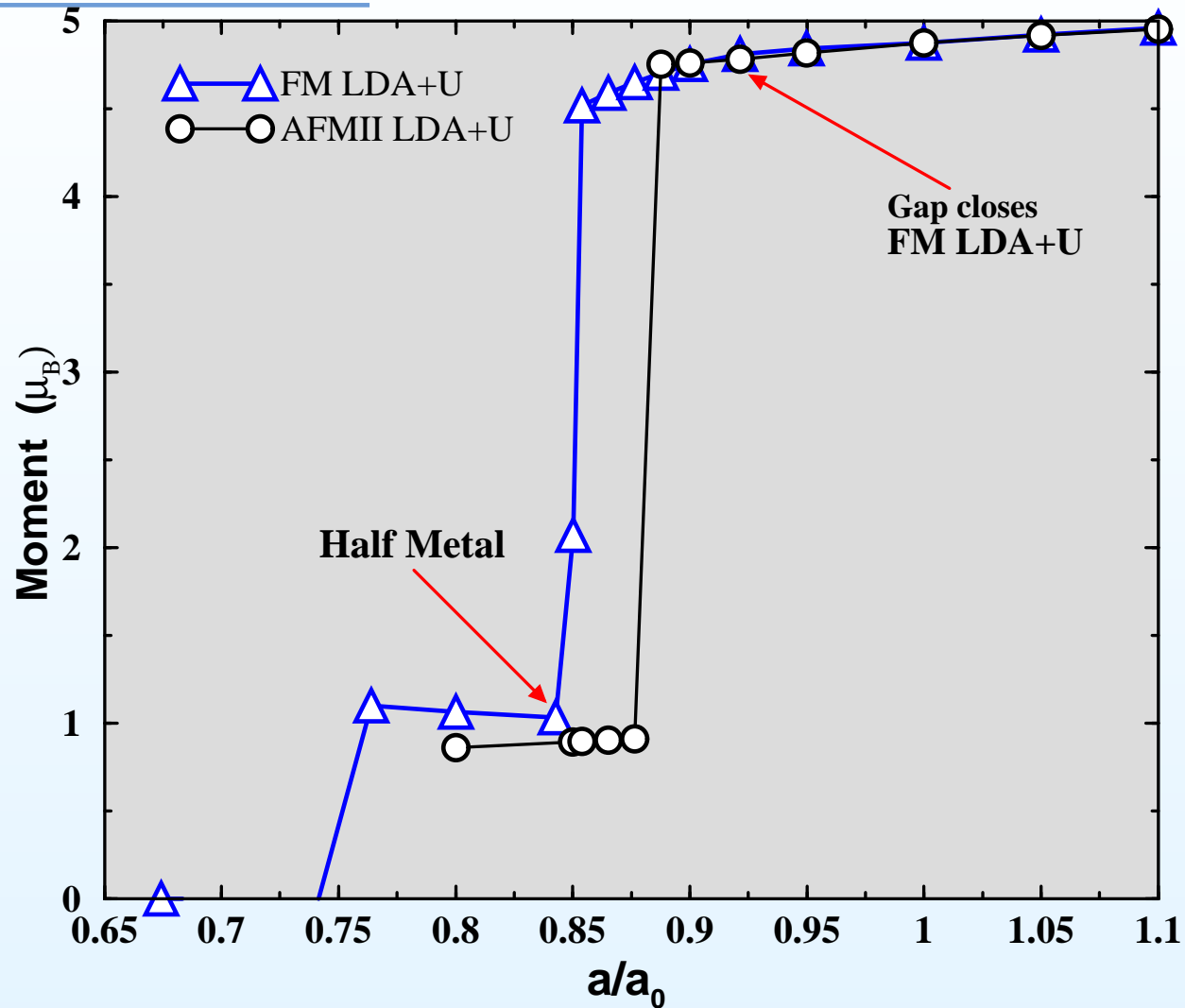
- Expt. → At 100-110 GPa, a  $\approx$  6.6% volume collapse with significant loss of moment (C.S.Yoo *et al.*, PRL 2005)

# Density of States



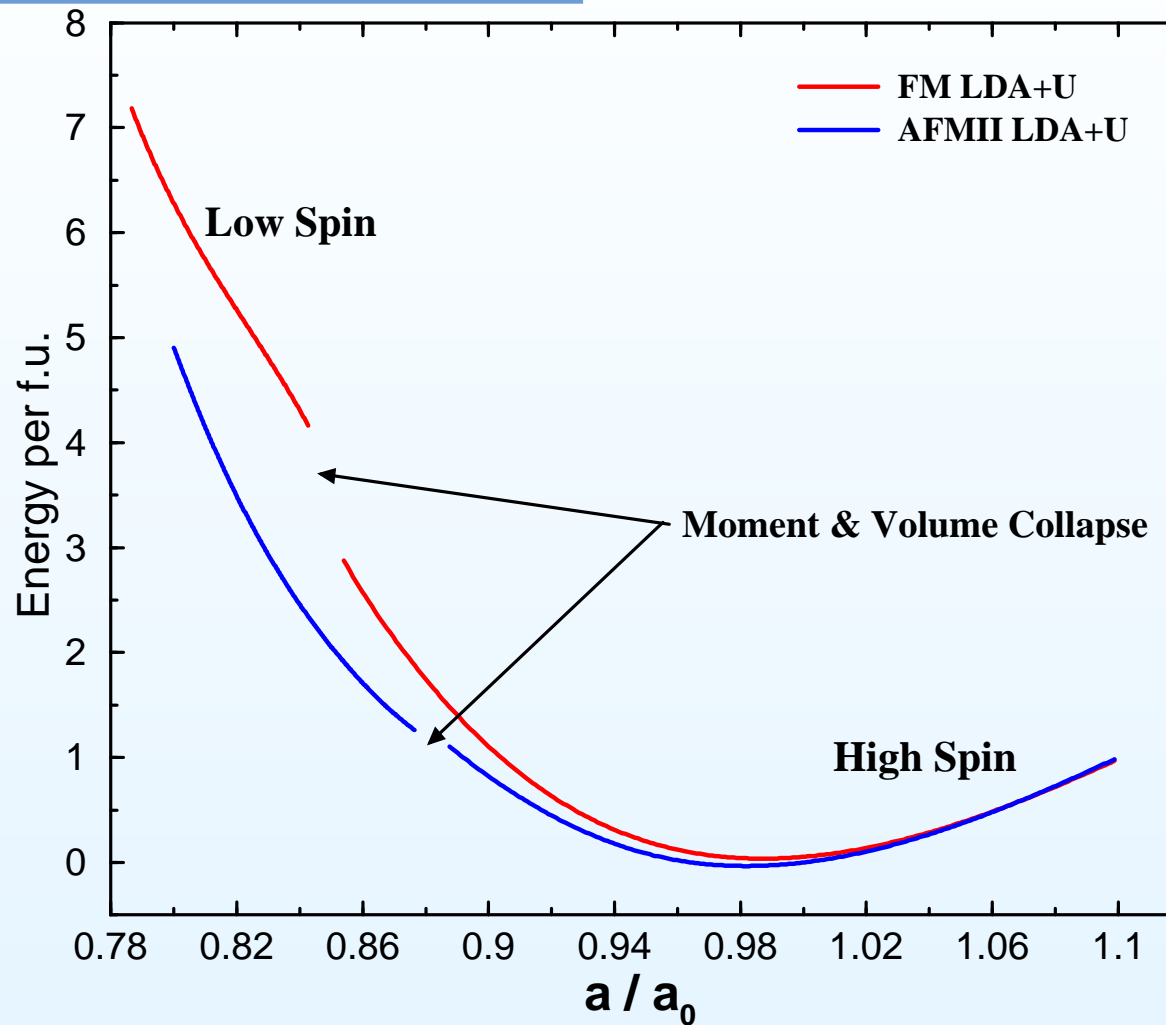
- Bandgap increases from 2.7 eV to 3.8 eV
- Before Collapse : 5 d orbitals singly occupied; spin moment  $\approx 5\mu_B$
- After Collapse : Two  $e^-$  from  $m = \pm 1$  doublet flip; spin moment  $\approx 1\mu_B$
- Both cases, total  $L = 0$

# FM & AFMII comparison



- AFMII → 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

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- 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))