Verwey transition in $Fe_3O_4$ investigated using LDA+ DMFT

L. Craco, M. S. Laad, and E. Muller Hartmann
presented by Soumen Bag

IISc, Bangalore

1 Sept, 2016
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At high temperature it has FCC lattice with two formula unit in the basis.

Verwey, Nature, 1939

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- Verwey transition at 122K(\( T_v \)).
- conductivity jump by factor of 100 across \( T_v \).
PES support insulator to insulator transition

D. Schrupp et al. EPL 2005
soft X-ray photo-emission data shows jump in the spectral onset energy across $T_v$

inset shows hysteresis during cooling and heating.

it shows spectral weight transfer (SWT) from low energy to high energy.

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What else associated with this transition?

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- $\text{Fe}^{3+} \text{Fe}^{3+,2+}_2 \text{O}_4$.
- Does B sublattice having charge order-disorder transition across $T_V$?
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- Does B sublattice having charge order-disorder transition across $T_{V}$?
- Does $\text{Fe}_{3} \text{O}_{4}$ go through structural transition and that changes the gap?
will there be charge order?

\[ \text{x-ray resonant scattering} \] show absence of CO along the c axis with the periodicity of either the cubic lattice q (001) or the doubled cubic lattice q (001/2). \textit{PhysRevLett.93.156408(2004)}
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✗ above result was strongly opposed by Joaquin Garcia, Phys. Rev. Lett. 109, 049701(2012)
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Theoretical Finding
The Fermi level crosses only the minority spin energy bands, consisting of spin-up t$_{2g}$ orbitals on the Fe B sublattice. A and B are Antiferromagnetically ordered.

The spin-polarized calculations high-temperature phase is a half metallic ferrimagnet, which is experimentally not observed. It’s a d electron, expected to be localised electron. Let’s see what happen after including Hubbard U for d orbitals.

V.N. Antonov et al. PRB 65, 134410(2001)
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LMTO data
In LDA+U approach Energy functional look like.

\[
E = E_{\text{LDA}} + \sum_I \left[ \frac{U_I}{2} \sum_{m,\sigma \neq m',\sigma'} n_{m'}^{\sigma'} n_m^{\sigma} - \frac{U_I}{2} n_I (n_I - 1) \right] \quad (1)
\]

where

\[
n_{m,m'}^{I\sigma} = \sum_{k,\nu} f_{k,\nu}^{\sigma} \langle \psi_{k,\nu}^{\sigma} | \phi_{m'}^I \rangle \langle \phi_{m}^I | \psi_{k,\nu}^{\sigma} \rangle \quad (2)
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\[ n^l_{m, m'} = \sum_{k, \nu} f^\sigma_{k, \nu} \langle \psi^\sigma_{k, \nu} | \phi^l_{m'} \rangle \langle \phi^l_{m} | \psi^\sigma_{k, \nu} \rangle \] (2)

Hubbard corrective potential on the Kohn-Sham wave functions needed for the minimization process

\[ V | \psi^\sigma_{k, \nu} \rangle = V_{LDA} | \psi^\sigma_{k, \nu} \rangle + \sum_{l, m} U^l \left( \frac{1}{2} - n^l_{m, \sigma} \right) | \phi^l_{m} \rangle \langle \phi^l_{m} | \psi^\sigma_{k, \nu} \rangle \] (3)
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the Hubbard potential is repulsive for less than half-filled orbitals \( n_{m}^l < \frac{1}{2} \), attractive for the other.
LSDA+U

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The difference between the potential acting on occupied and unoccupied states (whose size is of the order of \(U\)) also gives a measure of the energy
LSDA + U of high temperature cubic structure (Fd-3m)

Figure: Electron minority spin density of states

Przemyslaw Piekarz, PRL 97, 156402 (2006)
LSDA + U of high temperature cubic structure (Fd-3m)

$U = 4 \text{ eV and } J = 0.8 \text{ eV}$

- The spin-polarized calculations high-temperature phase is a half metallic.
- Now on I will be only focusing on minority spin sector across $E_F$

Figure: Electron minority spin density of states

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LSDA + U of low temperature monoclinic structure (P2/c)

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The spin-polarized calculations high-temperature phase (Fd\(\bar{3}m\)) is a half metallic phonon modes of \(\Delta_5\) and \(X_3\) (for details Ref.)

Low temp phase is insulating with gap 0.35 eV which is large compared to what experimentally observed.

What happen if we go beyond Hartee-Fock correction in local U?

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L. Craco, M. S. Laad, and E. Muller Hartmann, Verwey transition in Fe\(_3\)O\(_4\) investigated using...
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**Figure:** Electron minority spin density of states
Effective low energy Hamiltonian

Effective low energy model for $\text{Fe}_3\text{O}_4$.

$$H = \sum_{k\alpha\sigma} \epsilon_k c_{k\alpha\sigma}^a c_{K\sigma}^a + U \sum_{ia} n_{i\uparrow}^a n_{i\downarrow}^a + U' \sum_{iab} n_i^a n_i^b + V \sum_{\langle ij \rangle ab} n_i^a n_j^b - J_H \sum_{iab} S_i^a S_i^b + \Delta \sum_{i\sigma} (n_{i\sigma}^{A_{1g}} - n_{i\sigma}^{E_{g1}})$$

(4)

- $\epsilon_k$ the one electron band dispersion of $\text{Fe}(B)$-t2g, act as a bath in DMFT. Note that we will do DMFT on minority spin sector only.
- $a, b$ label the $A_{1g}, E_{g1}$ orbitals. under Jahn Teller(JT) t2g orbital split into doublet $E_{g1}$ and signlet $A_{1g}$ with LDA value of $\Delta=0.019\text{ev}$
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- from constrained LDA $U=4.1$ev, $U'=1.7$ev, $V=0.4$ev, $J_{H}=1.0$ev
- In single site DMFT we will decouple V in the HF approximation.
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- In single site DMFT we will decouple \( V \) in the HF approximation.
Instead of adding constant potential we will add frequency dependent self energy.

\[ G_a^{-1}(w) = [G_a^0(w)]^{-1} - \Sigma_a(w) \]  \hspace{1cm} (5)

\[ G_a(w) = \frac{1}{N} \sum_k \frac{1}{w + \mu - \Sigma_a(w) - \epsilon_{k\sigma}} \]  \hspace{1cm} (6)
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where \( \epsilon_{k\sigma} \) LSDA dos of t2g B sublattice orbital. self energy is given by

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where \( A_{ab} \) and \( B_{ab} \) are choose to get the atomic limit solution and free electron limit and

\[ \Sigma_{ab}^{(2)} = N_{ab} \frac{U_{ab}^2}{\beta^2} \sum_{lm} G_a^0(iw_l) G_b^0(iw_m) G_b^0(iw_l + iw_m - iw) \]  \hspace{1cm} (8)
\[ H = \sum_{k\alpha\sigma} \epsilon_k^a c_k^a c_\sigma^a + U \sum_{ia} n_i^a \uparrow n_i^a \downarrow + U' \sum_{iab} n_i^a n_i^b + V \sum_{(ij)ab} n_i^a n_j^b - J_H \sum_{iab} S_i^a S_i^b + \Delta \sum_{i\sigma} (n_{i\sigma}^{A1g} - n_{i\sigma}^{E_{g1}}) \]

(9)

orbital correlations and associated Jahn-Teller (JT) effects in a fully magnetically polarized situation might be essential ingredients for understanding the Verwey transition.
Results

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- Up to critical value \(\Delta_c = 0.01\) of the crystal-field splitting, all curves lie essentially on the one corresponding to the high-T phase.
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- For \( \Delta > \Delta_c \), however, we clearly see that all the curves seem to collapse onto the result for the low-T phase.

- Appreciable changes in dynamical SWT occur across \( \Delta_c \).

- Implies that the charge gap increases rapidly as \( \Delta \) is raised above \( \Delta_c \).
$A_{1g} \equiv (xy+yz+zx)$

- red line corresponds to low temperature.
- Blue corresponds to High T solution.
Results

- $A_{1g} \equiv (xy+yz+zx)$
- The red line corresponds to low temperature. Blue corresponds to High T solution.
- $E_{g1} \equiv (2xy-yz-zx), (xy-yz)$.
- $E_{g1}$ shows small change while $A_{1g}$ shows noticeable change. But both indicate the insulating state.
Comparison with experimental results

- $Gap_{LT} = 0.087 \text{ ev}$  $Gap_{HT} = 0.051 \text{ ev}$
- $\rho = \exp\left(\frac{Gap}{K_B T}\right)^4$. The across the array transition jump is 90. Exp velu is 100.
- Their calculation does not require the explicit inclusion of charge order CO within DMFT.
Author propose that B-site JT distortions in a correlated multiorbital situation play a crucial role in understanding the changes in electronic structure across the Verwey transition in Fe₃O₄.

In the strongly correlated situation, small changes in the B-site octahedral distortions with T give rise to large changes in dynamical spectral weight transfer from low to high energies, which is captured in LDA+DMFT.
Thanks to Prof. H.R. Krishnamurthy, Prof. Manish Jain, Prof. Anil Kumar for useful Discussion.
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Thank You all