Lattice instabilities of correlated electron materials and the topological Fermi surface transition in FeSe

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Effects of Parity Mixing in Correlated Electron Systems
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Main objective:

Understand the influence of electronic correlations on the structural stability of solids

Outline:

- Stabilization of paramagnetic bcc Fe by electronic correlations
- Structural instability near the MIT in $V_2O_3$
- Correlation-induced topological Fermi surface transition in FeSe upon lattice expansion
Until recently:

Theoretical investigations of electronic correlations in models and materials only for given lattice structure

Do strong correlations between the electrons affect the stability of the ionic lattice?

Electronic + ionic degrees of freedom:
Particularly difficult many-body problem: How to solve?
Collaborators:  Ivan Leonov (Augsburg)

Alexander Poteryaev
Sergey Skornyakov
Vladimir Anisimov

Yekaterinburg (Russia)
A reminder: Stabilization of paramagnetic bcc Fe by electronic correlations

DFT(GGA): paramagnetic bcc Fe is unstable

GGA+DMFT: paramagnetic bcc Fe is stabilized by electronic correlations

$T_{\text{struct}} \approx 1.3 \ T_C$

Leonov et al., PRL 106, 106405 (2011)
Lattice dynamics of paramagnetic $\text{bcc}$ iron

Non-magnetic GGA: Phonon dispersion

Exp.: Neuhaus, Petry, Krimmel (1997)

1. Brillouin zone

Dynamically unstable + elastically unstable ($C_{11}, C' < 0$)

Exp.: Neuhaus, Petry, Krimmel (1997)
Lattice dynamics of paramagnetic bcc iron

- implementation with plane-wave pseudo-potentials
- phonon frequencies calculated using frozen phonons
- harmonic approximation

GGA+DMFT: Phonon dispersion at 1.2 $T_C$

Coulomb interaction between Fe 3d electrons: $U_{mm'} = 1.8 \text{eV}$, $J = 0.9 \text{eV}$

Calculated:
- equilibrium lattice constant $a=2.883 \text{Å}$ ($a_{\text{exp}}=2.897 \text{Å}$)
- Debye temperature $\Theta=458 \text{ K}$

Leonov et al., PRB 85, 020401(R) (2012)

Paramagnetic bcc Fe: Phonons stabilized by electronic correlations

Exp.: Neuhaus, Petry, Krimmel (1997)
Structural instability near the Mott metal-insulator transition in $V_2O_3$
Phase diagram and electronic structure of $\text{V}_2\text{O}_3$

Electronic structure - $\text{V}^{3+} (3d^2)$: $S = 1$

McWhan et al. (1973)

Mott MIT $\leftrightarrow$ abrupt expansion by $\Delta V/V = 1.3\%$
Metal-insulator transition vs. structural transition in V$_2$O$_3$

- GGA implementation with plane-wave pseudo-potentials
- Calculate GGA+DMFT total energy as function of volume using exp. atomic positions and c/a ratio for PM V$_2$O$_3$
  \[ \text{PI } (V_{0.962\text{Cr}_{0.038}})_{2}\text{O}_3 \]

Correlations strongly redistribute charge density $\rightarrow$ need “charge self-consistency”

\[ \text{Coulomb interaction between V 3d electrons: } U_{\sigma\sigma'}^m : \bar{U} = 5.0\text{eV}, \; J = 0.93\text{eV} \]

\[ T = 390 \text{ K} \]

Leonov et al., PRB 91, 195115 (2015)

BUT:

PI phase (□) has lower energy, i.e., is stable, at ambient pressure $\rightarrow$ inconsistent with experiment (PM!)

Structural transition and MIT are decoupled

\[ \text{Energy (eV/f.u.)} \]

\[ \text{Volume (a.u.}^3) \]

\[ \text{PI} \]

\[ \text{PM} \]
Metal-insulator transition vs. structural transition in $\text{V}_2\text{O}_3$

- GGA implementation with plane-wave pseudo-potentials
- Calculate GGA+DMFT total energy as function of volume using exp. atomic positions and $c/a$ ratio for
  PM $\text{V}_2\text{O}_3$
  PI $(\text{V}_{0.962}\text{Cr}_{0.038})_2\text{O}_3$

![Charge self-consistent](image)

Structural transition and MIT are decoupled:
- Structural transition at $\Delta V / V = 1.5\%$ ($p_{\text{struct}} = -28$ kbar)
- Anomaly in the total energy near structural transition:
  volume collapse by 0.5% $\rightarrow$ divergence of compressibility

Coulomb interaction between V 3d electrons: $U_{nn'}: \bar{U} = 5.0eV, J = 0.93eV$

$T = 390$ K

Leonov et al., PRB 91, 195115 (2015)

Exp: Pfauser et al. (2006)
Exp: Populoh et al. (2011)

Correlation effect!
Metal-insulator transition vs. structural transition in V$_2$O$_3$

- GGA implementation with plane-wave pseudo-potentials
- Calculate GGA+DMFT total energy as function of volume using exp. atomic positions and c/a ratio for
  PM V$_2$O$_3$
  PI (V$_{0.962}$Cr$_{0.038}$)$_2$O$_3$

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\[ U_{\text{nnn}}^{\sigma\sigma'} = 5.0eV, \quad J = 0.93eV \]

$T = 390$ K

Leonov et al., PRB 91, 195115 (2015)

“Breakdown of Hooke’s law”:
Zacharias, Bartosch, Garst (2012)
M. Lang (this meeting)

Exp: Pfalzer et al. (2006)
Exp: Populoh et al. (2011)
Orbital-selective behavior

- $a_{1g}$ orbitals: quasiparticle weight $Z$ remains finite
- $e_{g}^{\pi}$ orbitals: $Z \to 0$ ($m^*/m$ diverges) $\rightarrow$ Brinkman-Rice transition!

Coulomb interaction between V 3d electrons: $U_{nn'}^{\sigma\sigma'}: \bar{U} = 5.0 eV, J = 0.93 eV$

$T = 390 K$

Leonov et al., PRB 91, 195115 (2015)
Correlation-induced topological Fermi surface transition in FeSe upon expansion
Fe-based superconductors

Layered structure, but no separating layers

Superconductivity induced by doping or pressure

Effects of parity mixing may be observable
FeSe: Crystal structure and properties

- Tetragonal crystal structure
- $T_c = 8$ K (37 K under hydrostatic pressure)
- Isovalent substitution Se → Te (lattice expansion) → $T_c$ increases up to 14 K

Superconductivity above 100 K in single-layer FeSe films on doped SrTiO$_3$

Jian-Feng Ge$^1$, Zhi-Long Liu$^1$, Canhua Liu$^{1,2}$*, Chun-Lei Gao$^{1,2}$, Dong Qian$^{1,2}$, Qi-Kun Xue$^3$*, Ying Liu$^{1,2,4}$ and Jin-Feng Jia$^{1,2}$*

Origin: Lattice expansion and/or electron doping?
FeSe: Crystal structure and properties

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- $T_c = 8\, \text{K}$ (37 K under hydrostatic pressure)
- Isovalent substitution Se $\rightarrow$ Te (lattice expansion) $\rightarrow$ $T_c$ increases up to 14 K

<table>
<thead>
<tr>
<th></th>
<th>FeSe</th>
<th>FeSe$_{1-x}$Te$_x$, $x&lt;0.7$</th>
<th>FeTe</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>no static magnetic order, short-range fluctuations with $Q_m=(\pi, \pi)$</td>
<td>$T_N \sim 70, \text{K}$ $Q_m=(\pi, 0)$</td>
<td>-</td>
</tr>
<tr>
<td>$T_c$</td>
<td>$8, \text{K}$</td>
<td>$14, \text{K}$</td>
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- Why does the electronic and magnetic structure of FeSe change with lattice expansion?
- Why does $T_c$ increase?
FeSe: Phase stability and local magnetism

Coulomb interaction between Fe 3d electrons: \( U_{\alpha\alpha'} = 3.5 \text{eV}, J = 0.85 \text{eV} \)

- Isostructural transformation upon 10% expansion of the lattice \( (p_c = -6.4 \text{ GPa}) \)
- Strong increase of the fluctuating magnetic moment and compressibility

Left minimum \( a = 7.07 \text{ a.u.} \)  
Right minimum \( a = 7.35 \text{ a.u.} \)

\[
B = 70 \text{ GPa} \quad \sqrt{\langle \mu_z^2 \rangle} = 2 \mu_B \quad 35 \text{ GPa} \quad 3.25 \mu_B
\]

Observed in FeTe:
- tetragonal to collapsed-tetragonal phase transformation under pressure
- suppression of magnetism under 4-6 GPa

Exp: Zhang et al. (2009)
FeSe: Spectral function

Van Hove singularity shifts to $E_F$ due to correlations

Low-volume phase

Expansion

High-volume phase

T = 290 K

Leonov et al., PRL 115, 106402 (2015)
FeSe: Spectral function

Van Hove singularity shifts to $E_F$ due to correlations

Exp.: Yokoya et al. (2012)

Spectral weight suppressed with Te substitution ($=\text{lattice expansion}$)

Low-volume phase

Expansion

High-volume phase

$T = 290\, K$

Leonov et al., PRL 115, 106402 (2015)
FeSe: Electronic structure

Proposition:
Superconductivity in FeSe\textsubscript{1-x}Te\textsubscript{x} strongly influenced, or even induced, by Van Hove singularity

Low-volume phase:
- Renorm. of quasiparticle bands + orbital-selective shift
- Van Hove singularity at $M$ point pushed towards $E_F$

High-volume phase:
- Complete reconstruction of electronic structure
- Correlation-induced shift of Van Hove singularity above $E_F$

Shift of Van Hove singularity to $E_F$ goes along with increase of $T_c$ in FeSe\textsubscript{1-x}Te\textsubscript{x}

Leonov et al., PRL 115, 106402 (2015)
FeSe: Fermi surface

Low-volume phase:
- Correlations do not change FS
- In-plane nesting with $Q_m=(\pi, \pi)$

High-volume phase:
- Correlations change FS topology
- Lifshitz transition
- Electron pocket at $M$ point vanishes
- In-plane nesting with $Q_m=(\pi, 0)$

Correlation-induced change of magnetic structure upon lattice expansion

In accord with ARPES experiments on FeSe$_{1-x}$Te$_x$
Xia et al. (2009), Tamai et al. (2010), Maletz et al. (2014), Nakayama et al. (2014)
FeSe: Fermi surface

Experiment

Watson et al. arXiv:1603.04545v2

“Size of pockets smaller than in DFT”

GGA+DMFT

Leonov et al. (2016, unpublished)

... and than in DFT+DMFT?

Size of pockets changes with pressure along c axis → lattice optimization required
Conclusion:

Electronic correlations in the solid can strongly influence the structural stability of materials.