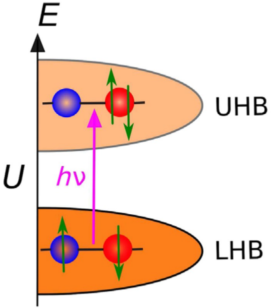
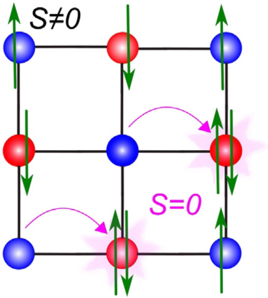
Correlations and Hubbard model

Mott insulator and Mott transition



Phys. Rev. X 9, 021020 (2019)



by Alexander Tsirlin, Leipzig University

Lecture 18: January 13, 2025

Exam: 17.02, 9:00 (kleiner Hörsaal)

Second exam: 24.03, 9:00 (SR 218)

Exam: 17.02, 9:00 (kleiner Hörsaal)

Second exam: 24.03, 9:00 (SR 218)

Exam problems:

– questions about the key concepts
  example: Berry curvature and its symmetry properties

– analytical problems
  example: tight-binding model

– numerical problems
  example: calculate effective mass from the experimental data

Condensed matter:
Theory should be on tap, not on top

Philip Anderson (1923–2020)

Condensed matter:
Theory should be on tap, not on top

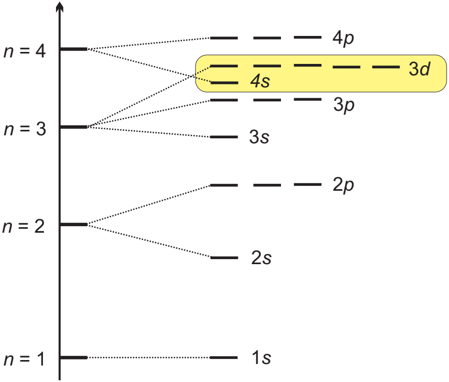
Philip Anderson (1923–2020)

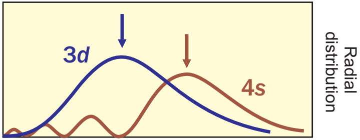
1977 Nobel prize in physics

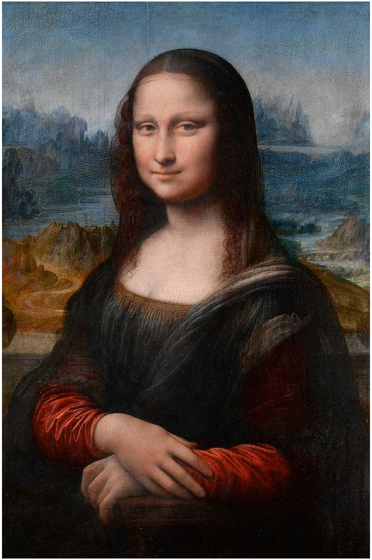
“for his investigations into the electronic structure of magnetic and disordered systems, which allowed for the development of electronic switching and memory devices in computers”

Correlated states: Localized shells

Image credit: WNYC New York Public Radio (CC-BY-NC)


n = 4
n = 3
n = 2
n = 1
4p
3d
4s
3p
3s
2p
2s
1s


3d
4s
Radial distribution
Distance from the nucleus



viridian (Cr_2O_3)

red ochre (Fe_2O_3)

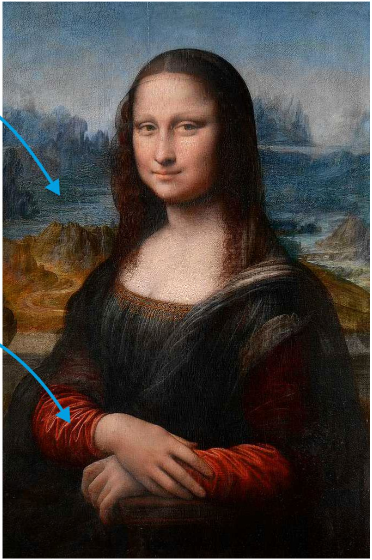
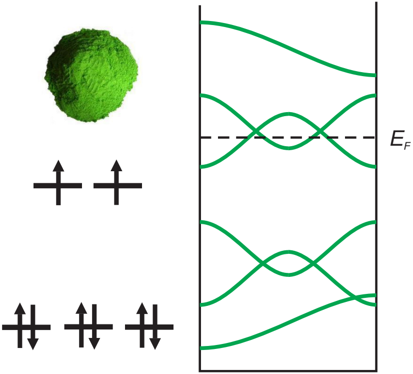


Image credits: Benjah-bmm27 and A,Ocram (CC-zero)

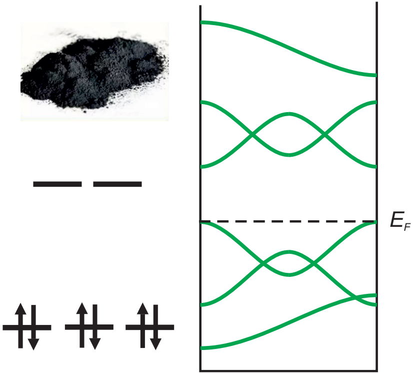
Mott-Hubbard

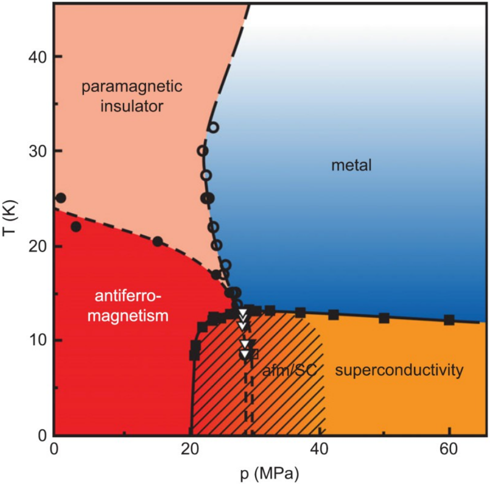
Kondo

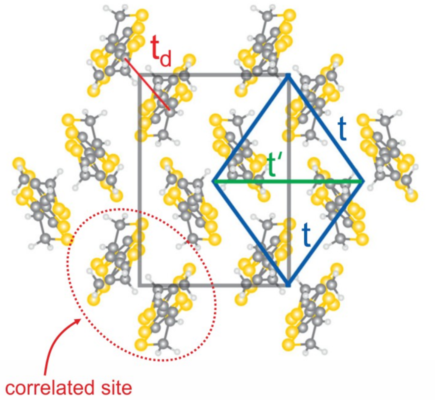


Mott insulator (NiO)

Band insulator ($LaCoO_3$)



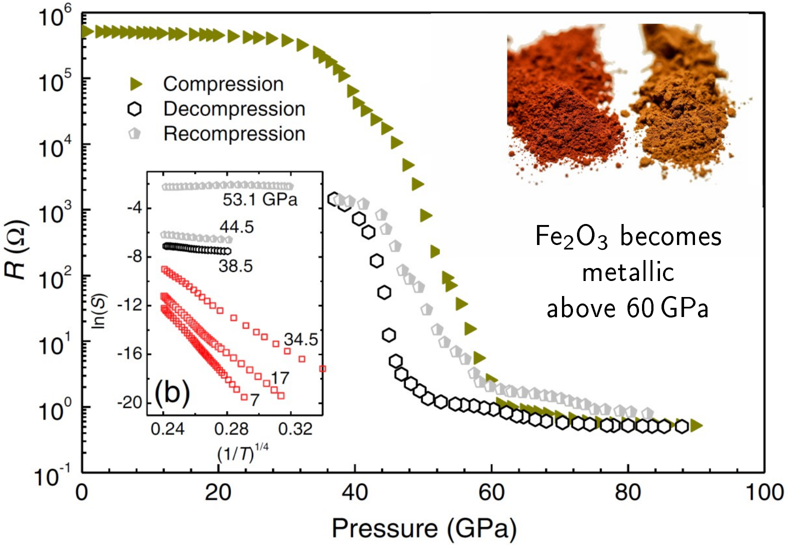




Charge-transfer salts: $t_d \sim 1\,\text{eV}$

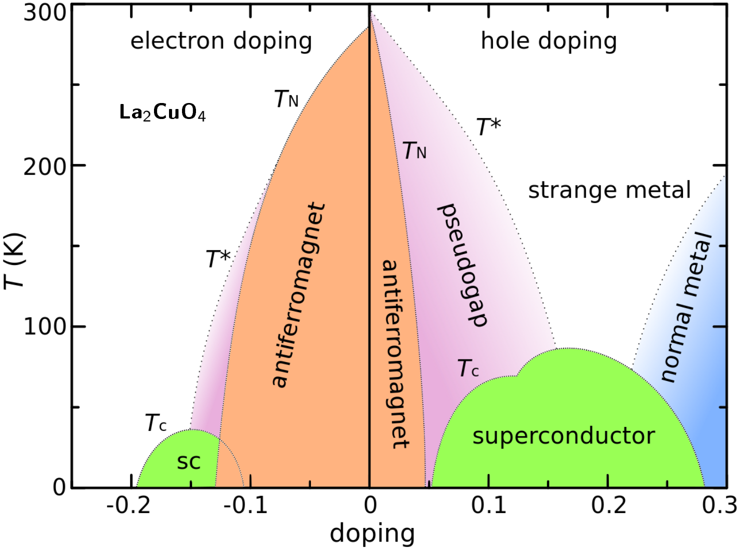
$t, t' \sim 0.05\,\text{eV}, \quad U \sim 0.1\,\text{eV}$

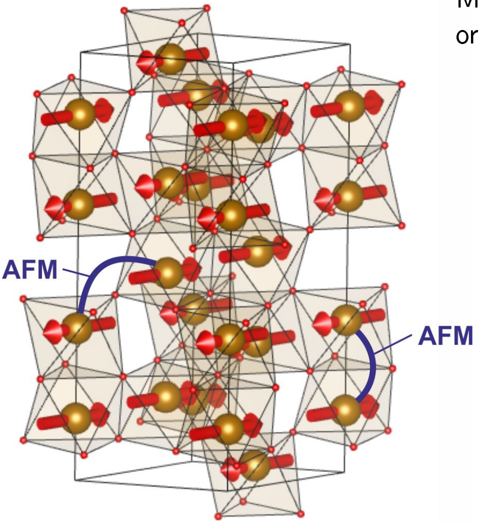
Adv. Phys. 69, 1 (2020)



Fe_2O_3 becomes metallic above 60 GPa

Phys. Rev. X 8, 031059 (2018)

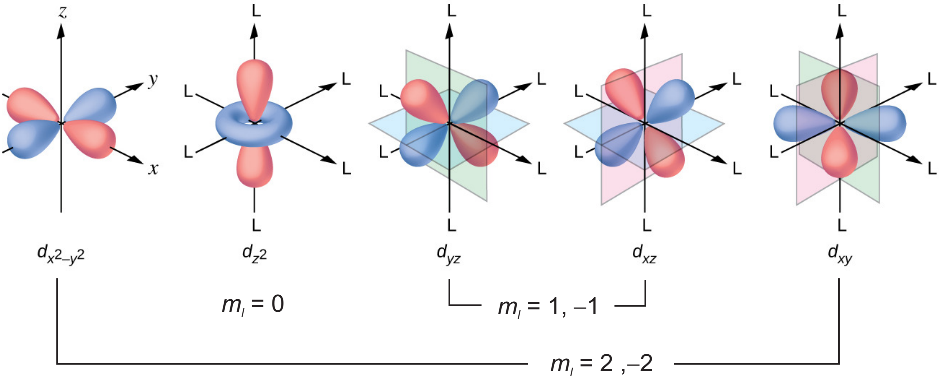

electron doping
hole doping
La2CuO4
TN
T*
TN
T*
strange metal
antiferromagnet
antiferromagnet
pseudogap
normal metal
Tc
Tc
sc
superconductor
300
200
100
0
T (K)
-0.2
-0.1
0
0.1
0.2
0.3
doping



Fe_2O_3

Mott insulators are magnetically ordered because of correlations

Image credit: Bilbao Crystallographic Server

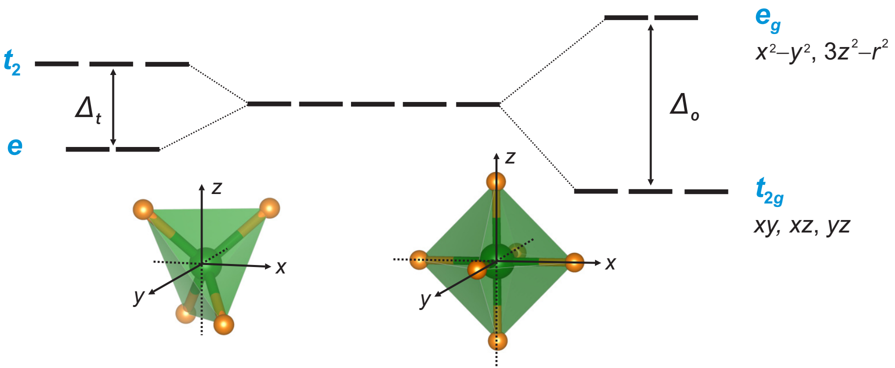


Spherical harmonics, $Y^l_m(\theta,\varphi)$, or their combinations:

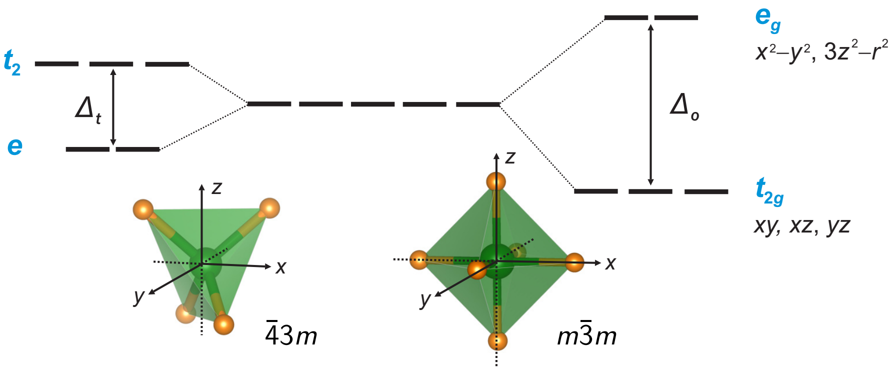
$$|3z^2 - r^2\rangle = Y^2_0$$

$$|x^2 - y^2\rangle = \frac{1}{\sqrt{2}}(Y^2_2 + Y^2_{-2})$$

...



t_2
Δ_t
e
e_g
$x^2–y^2$, $3z^2–r^2$
Δ_o
t_{2g}
xy, xz, yz
z
x
y
z
x
y



Crystal-field levels are labeled by irreducible representations of the symmetry group

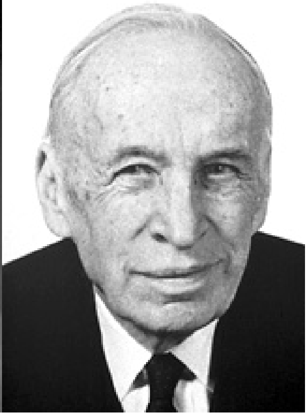
Ruby

Cr^{3+} in corundum, Al_2O_3

Emerald

Cr^{3+} in beryl, $Be_3Al_2Si_6O_{18}$

Correlated materials: 1977 Nobel prize in physics



Philip Anderson
1923–2020

Sir Neville Mott
1905–1996

John Van Vleck
1899–1980