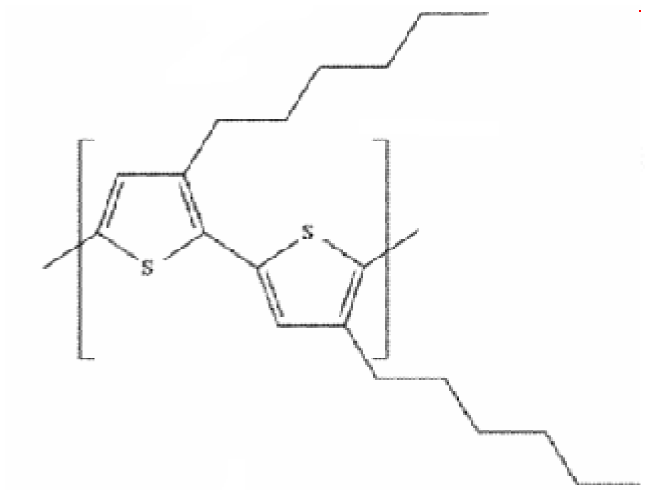
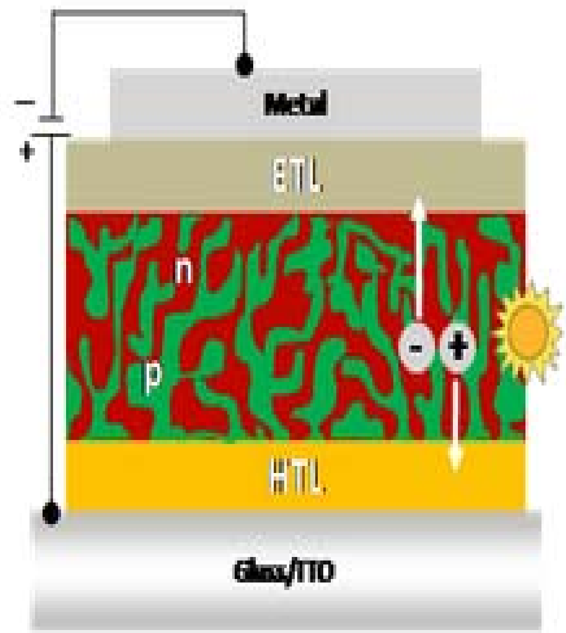
27. Quasiparticles

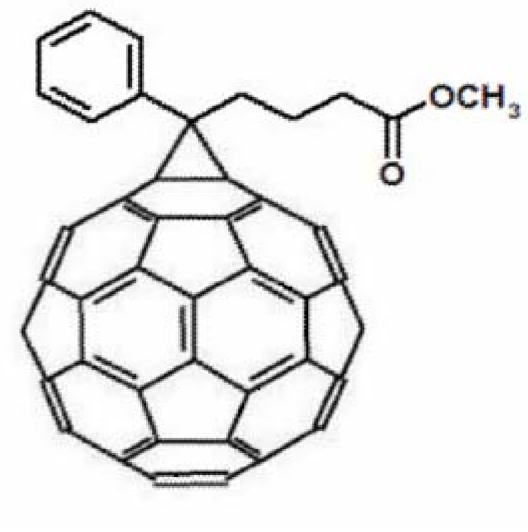
Jan. 24, 2018

Organic solar cells



P3HT donor





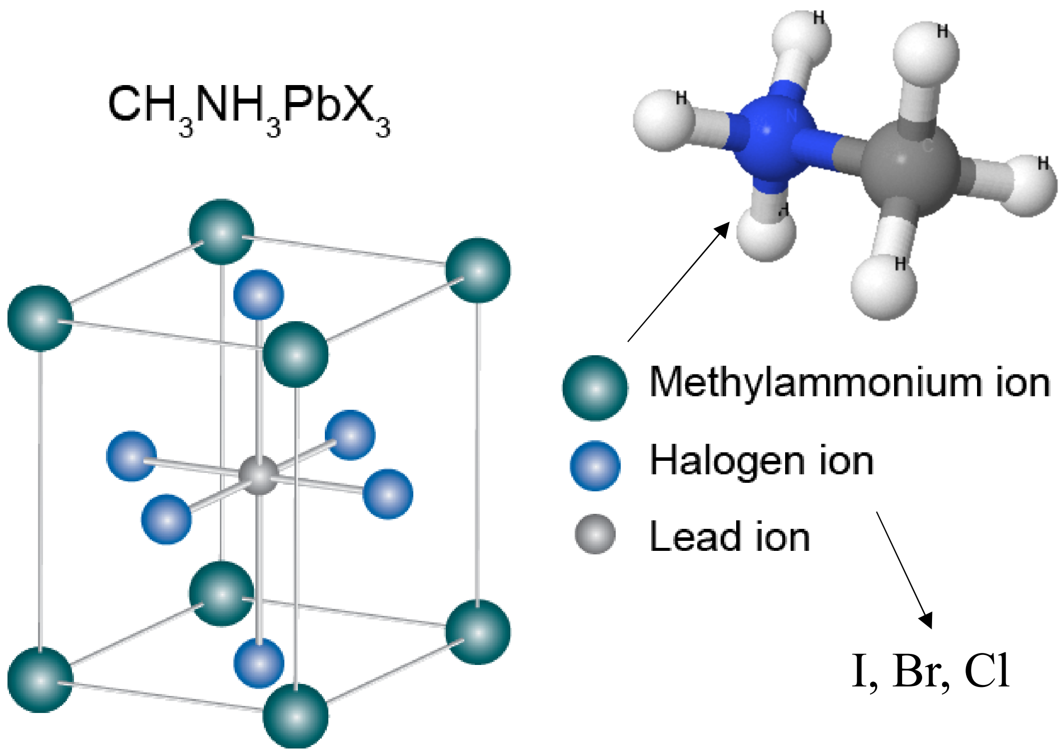
PCBM acceptor

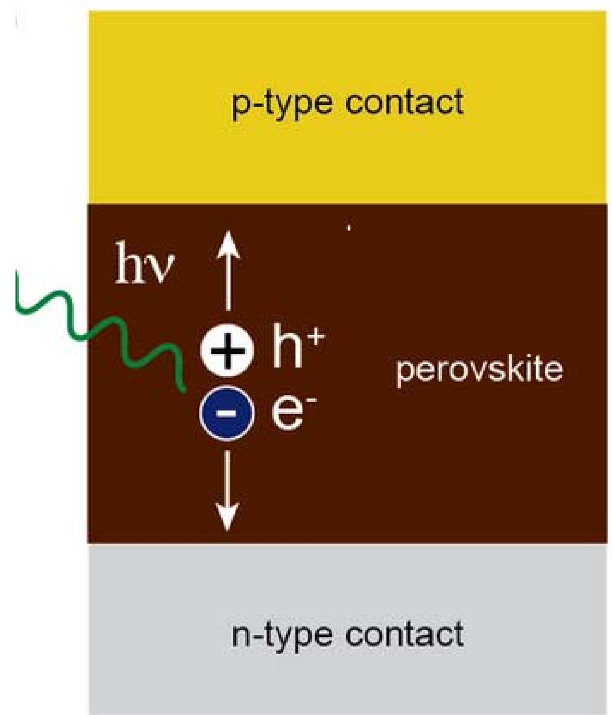
Excitons in polymers: a monomer is in an excited states and this moves down the chain.

https://www.uni-ulm.de/nawi/nawi-oc2/forschung/ag-organische-halbleiter-und-farbstoffe-fuer-die-photovoltaik.html?print=1

Perovskite solar cells

$CH_3NH_3PbX_3$



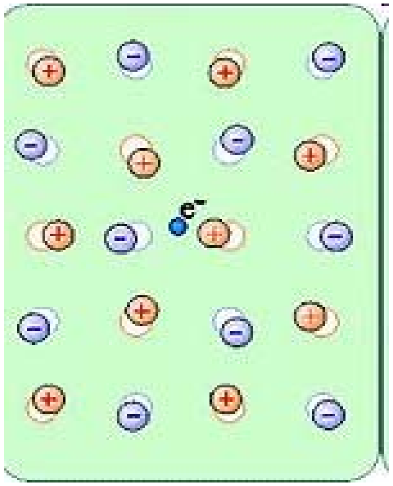


Efficiency ~ 22%

https://en.wikipedia.org/wiki/Perovskite_solar_cell

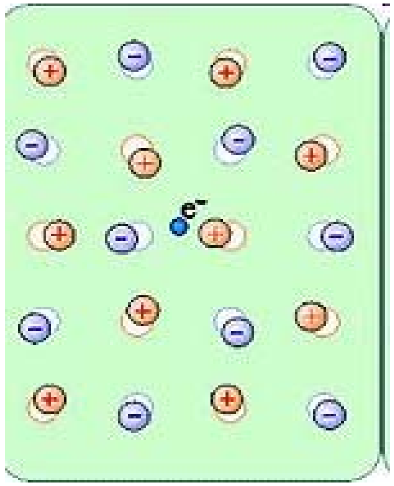
Polarons

A polaron is a quasiparticle consisting of an electron and an ionic polarization field. The electron density is low so the screening by electrons can be neglected.



Electronic charge is partially screened by lattice ions. This is a charge - phonon coupling.

Large polaron (Fröhlich polaron)



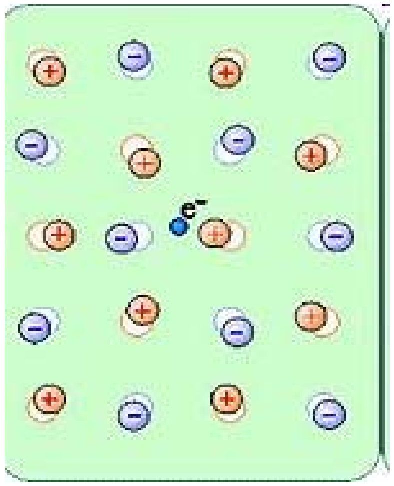
The spatial extent of the polaron is much larger than the lattice constant.

Large polarons typically form bands.

Electrons move in bands with a large effective mass (432 m_e for NaCl)

Small polaron (Holstein polaron)

For a small polaron, the polarization is about the size of the lattice contant.



Small polaron - Holstein Hamiltonian - electrons are localized and hop (thermally activated or tunneling). Small polarons often form in organic material. In soft materials the energy for making a distortion is smaller.

Bipolarons

Two polarons can bind together to form a bipolaron (a quasiparticle).

Elastic strain energy is reduced by sharing the polarization field.

Bipolarons have integral spin -> they are bosons.

It is possible that the condensation of bipolarons into the same ground state could lead to superconductivity.

Bipolarons

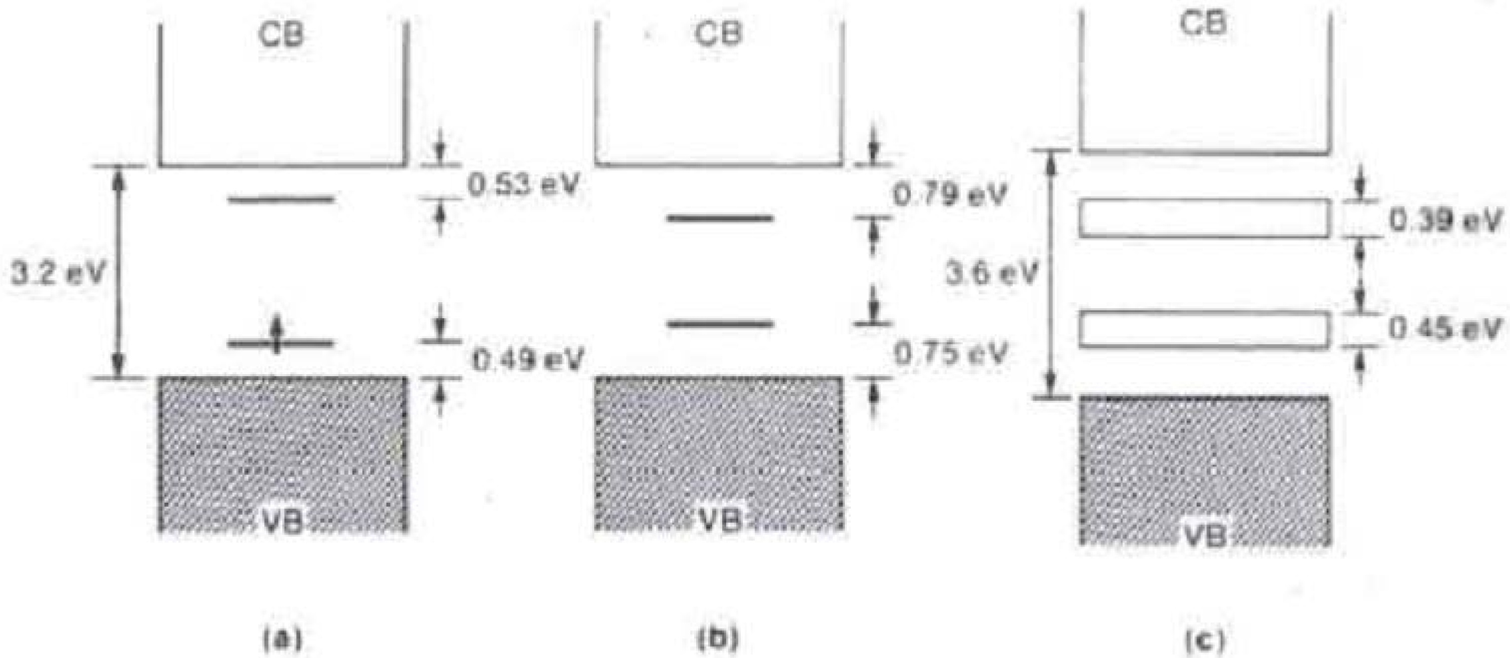


Figure 10. Evolution of the polypyrrole band structure upon doping: (a) low doping level, polaron formation; (b) moderate doping level, bipolaron formation; (c) high (33 mol %) doping level, formation of bipolaron bands.

J. L. Breda and G. B. Street, Acc. Chem. Res. 1985, 18, 309-315.

Landau theory of a Fermi liquid

If there are no electron-electron interactions, electrons have an infinite lifetime and the probability that a state is occupied is given by the Fermi function.

If there are interactions, quasiparticles have a finite lifetime. The lifetime can be calculated by Fermi's golden rule.

The occupation probability of a state depends on the occupation the other states. You solve for the probability distribution by solving a master equation. The occupation probability is not given by the Fermi function.

$$\Gamma_{k \to k'} = \frac{2\pi}{\hbar} \left| \langle \psi_k | H | \psi_{k'} \rangle \right|^2 \delta\left(E_k - E_{k'} \right)$$

Landau theory of a Fermi liquid

The free electron model = 'Fermi gas' is very successful at describing metals but it is not clear why this is so since electron-electron interactions are completely ignored.

Landau first considered the "normal modes" of an interacting electron system. The low lying excitations he called quasiparticles.

The quasiparticles have as many degrees of freedom as the electrons. They can be labeled by k.

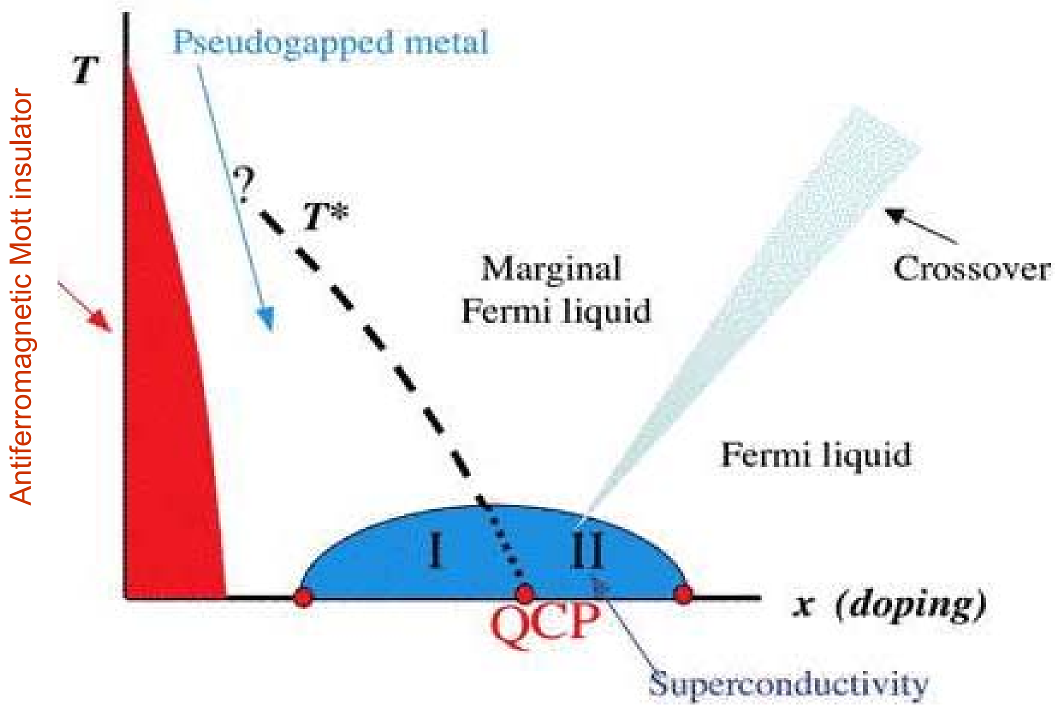
Quasiparticles can be have the same spin, charge, and k vectors as the electrons.

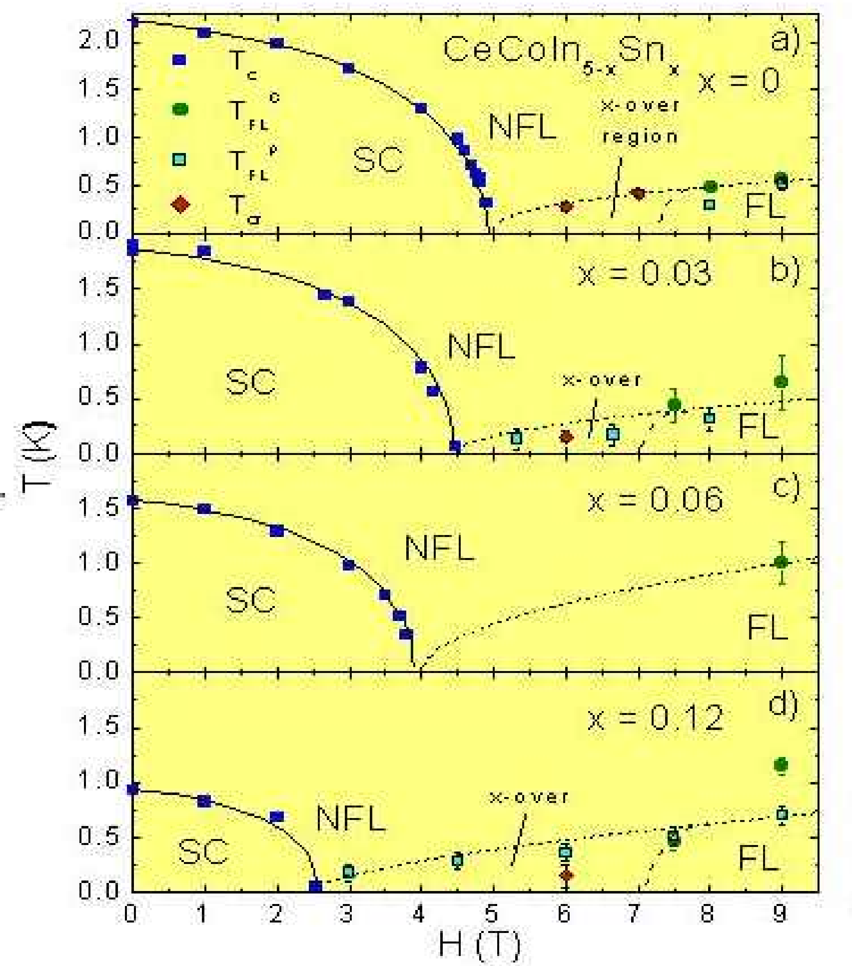
It is not easy to calculate $E(k)$.

Concepts like the density of states refer to quasiparticles.

Instabilities Fermi liquid

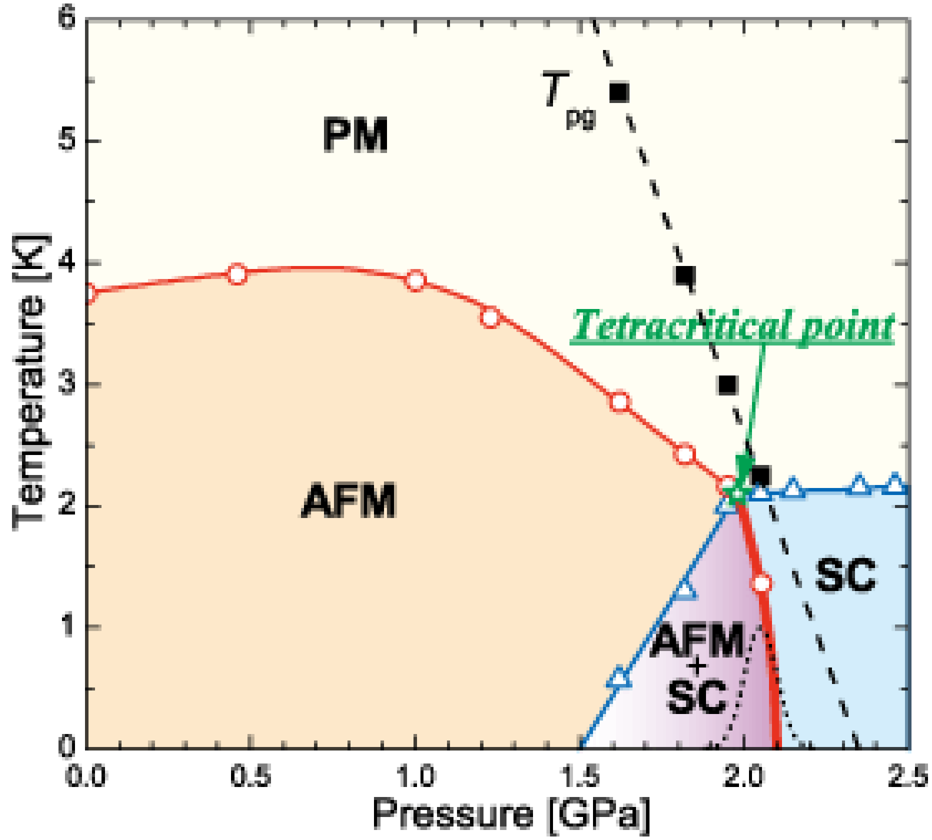
Some metals cannot be described as a Fermi liquid.





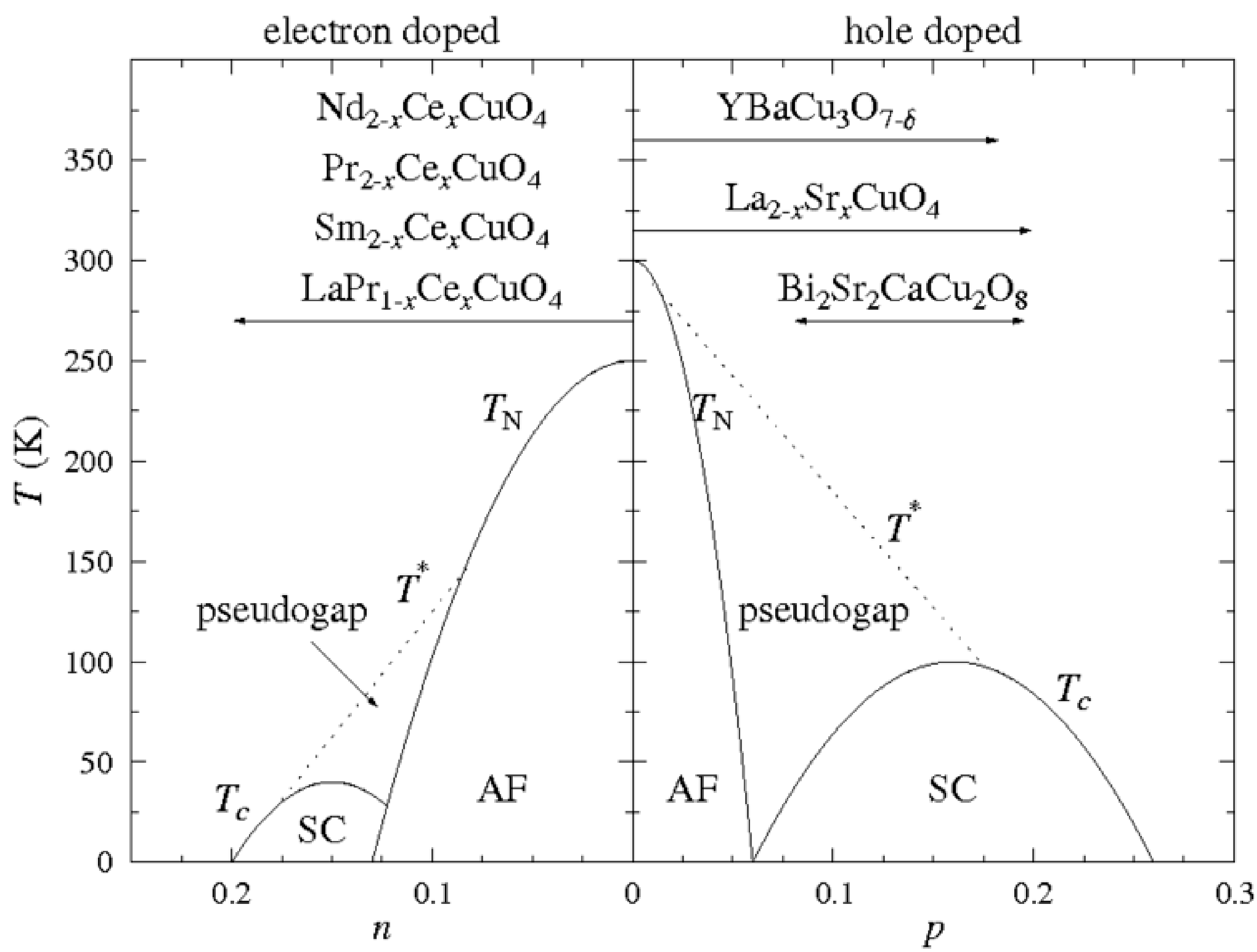
Heavy Fermion $CeCu_2Si_2$

Some metals cannot be described as a Fermi liquid.

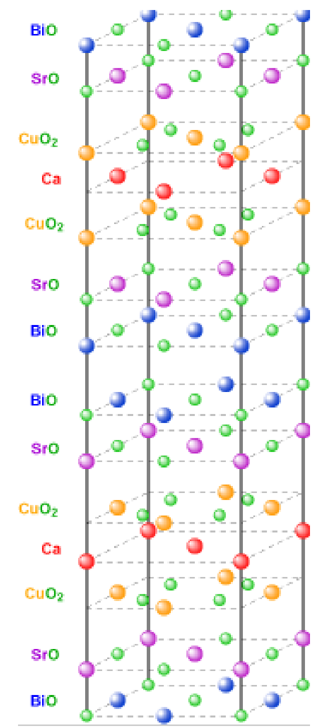


http://www.ipap.jp/jpsj/announcement/announce2007May.htm

Cuprate superconductors

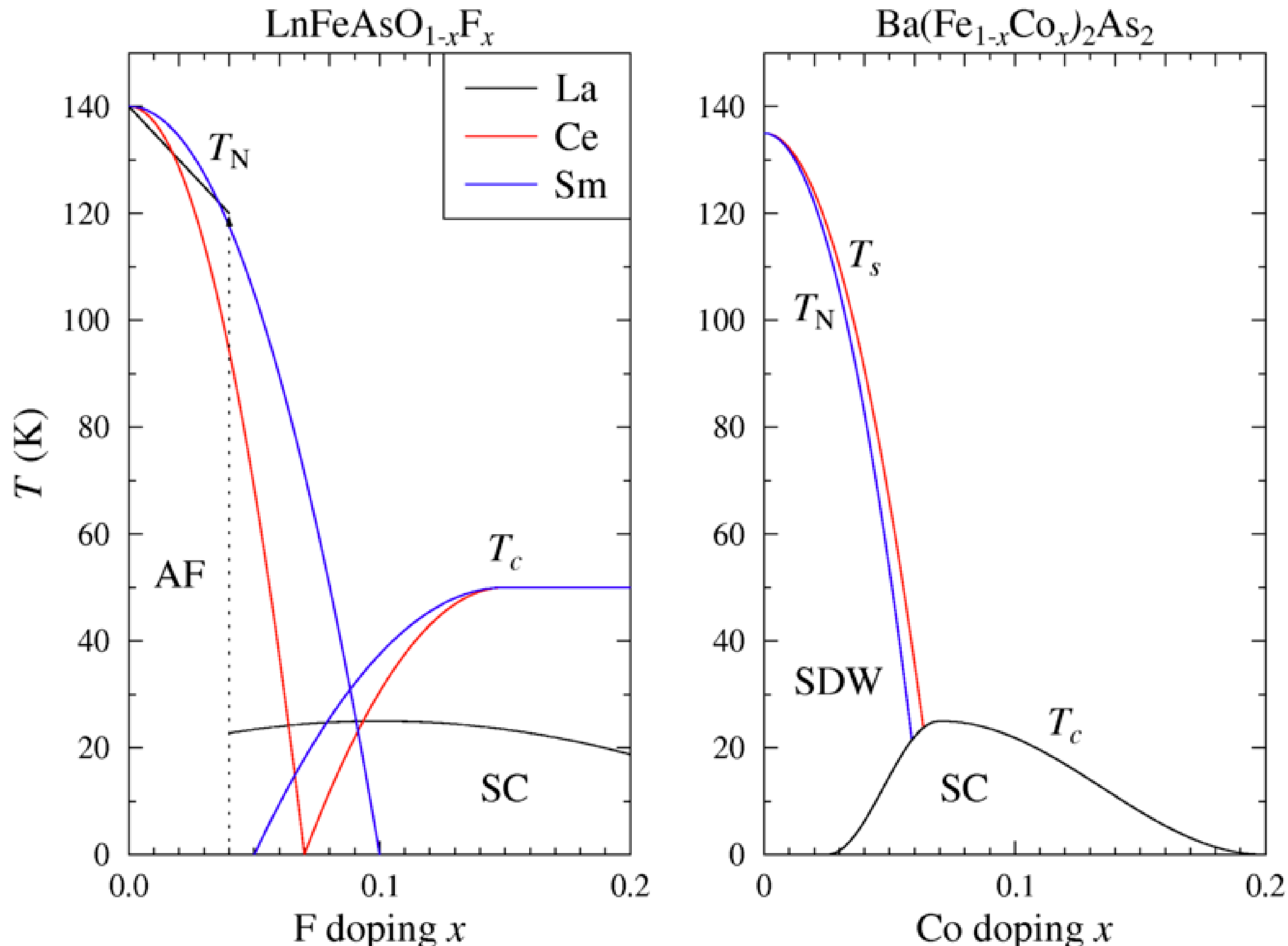


from Wikipedia



The unit cell of high-temperature cuprate superconductor BSCCO-2212

Iron based superconductors



from Wikipedia

Metal -Insulator Transitions Electron - Electron Interactions

Electron-electron interactions

Including electron-electron interactions into the description of solids is very, very difficult.

$$H = -\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_A \frac{\hbar^2}{2m_A}\nabla_A^2 - \sum_{i,A}\frac{Z_A e^2}{4\pi\varepsilon_0 r_{iA}} + \sum_{i<j}\frac{e^2}{4\pi\varepsilon_0 r_{ij}} + \sum_{A<B}\frac{Z_A Z_B e^2}{4\pi\varepsilon_0 r_{AB}}$$

One of the simplest approximation is to say that the electron-electron interactions screen the nuclei-electron interactions.

Screening = Abschirmung

Electron screening (Abschirmung)

$$\nabla \cdot \vec{E} = \frac{e\delta(r)}{\varepsilon_0} \qquad\qquad \vec{E} = -\nabla V$$

Poisson equation $$\nabla^2 V = -\frac{e\delta(r)}{\varepsilon_0} \qquad\qquad V = \frac{e}{4\pi\varepsilon_0 \left|\vec{r} - \vec{r}'\right|}$$

If a charge is put in a metal, the other charges will move

$$\nabla^2 V = -\frac{e\delta(r)}{\varepsilon_0} - \frac{\rho_{ind}}{\varepsilon_0}$$

If ρ_{ind} is proportional to -V,

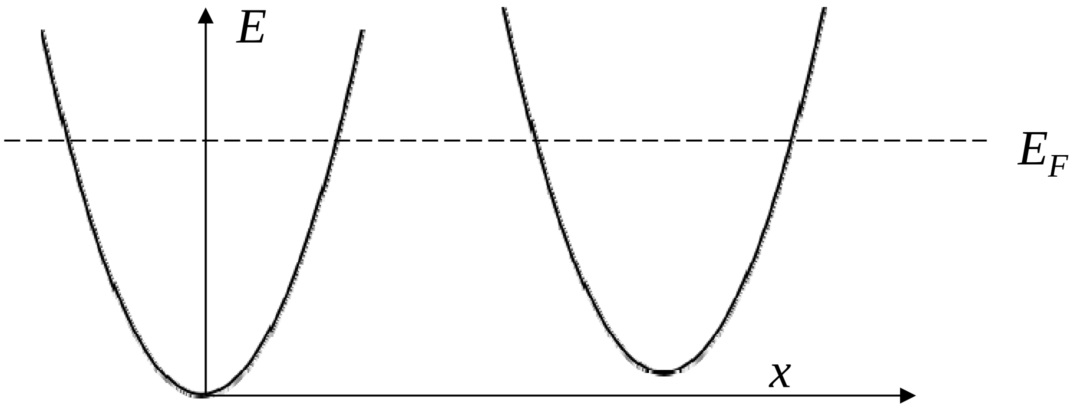
$$\frac{\rho_{ind}}{\varepsilon_0} = -k_s^2 V$$

The Helmholtz equation in 3-d

$$\nabla^2 V - k_s^2 V = -\frac{e\delta(r)}{\varepsilon_0}. \qquad\qquad V = \frac{e\exp\left(-k_s \left|\vec{r} - \vec{r}'\right|\right)}{4\pi\varepsilon_0 \left|\vec{r} - \vec{r}'\right|}$$

Thomas-Fermi screening

$$\Delta n = -D(E_F)eV$$



$$\rho_{ind} = e\Delta n = -e^2 D(E_F) V$$

$$D(E_F) = \frac{3n}{2E_F}$$

$$\nabla^2 V = -\frac{e\delta(r)}{\varepsilon_0} - \frac{\rho_{ind}}{\varepsilon_0} = -\frac{e\delta(r)}{\varepsilon_0} + \frac{3e^2 n}{2\varepsilon_0 E_F} V$$

$$\nabla^2 V - \frac{3e^2 n}{2\varepsilon_0 E_F} V = -\frac{e\delta(r)}{\varepsilon_0}$$

Thomas - Fermi screening length

$$k_s^2 = \frac{3e^2 n}{2\varepsilon_0 E_F} = \frac{3^{1/3} m e^2 n^{1/3}}{\varepsilon_0 \hbar^2 \pi^{4/3}}$$

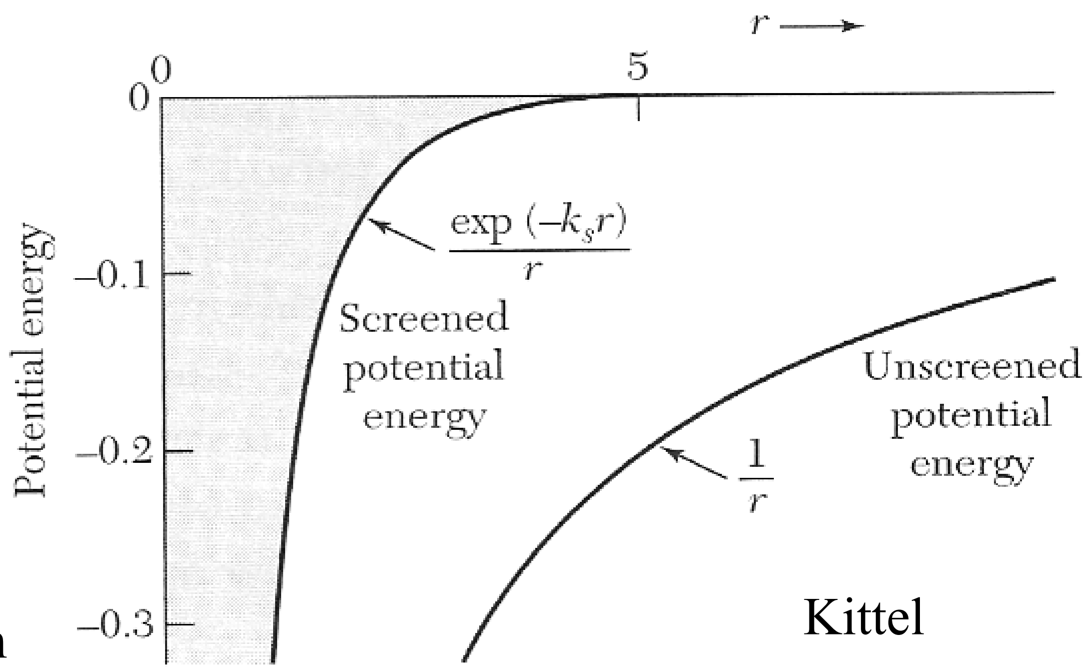
$$V = \frac{-e \exp\left(-k_s \left|\vec{r} - \vec{r}'\right|\right)}{4\pi\varepsilon \left|\vec{r} - \vec{r}'\right|}$$

Electron screening

$$V = \frac{-\exp\left(-k_s\left|\vec{r}-\vec{r}\,'\right|\right)}{4\pi\varepsilon\left|\vec{r}-\vec{r}\,'\right|}$$

$$k_s^2 = \frac{3e^2 n}{2\varepsilon_0 E_F} = \frac{3^{1/3} m e^2 n^{1/3}}{\varepsilon_0 \hbar^2 \pi^{4/3}}$$

Thomas - Fermi screening length



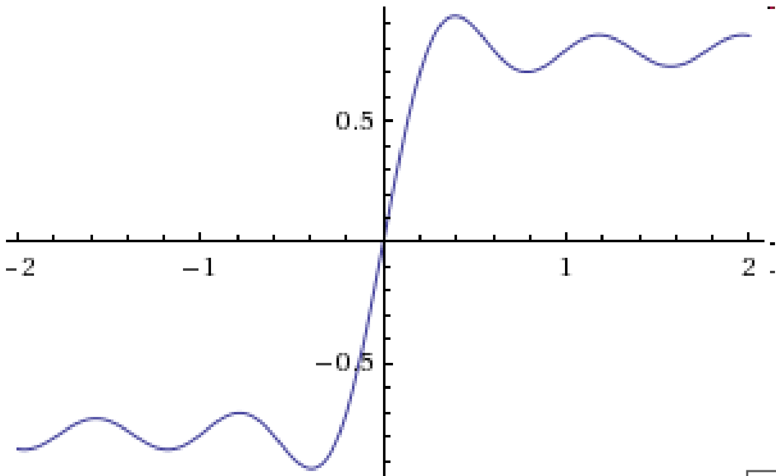
Kittel

$$k_s^2 \propto n^{1/3}$$

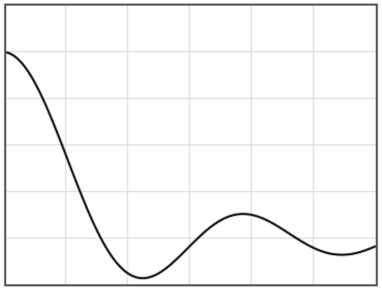
Screening length depends on the electron density

Friedel oscillations

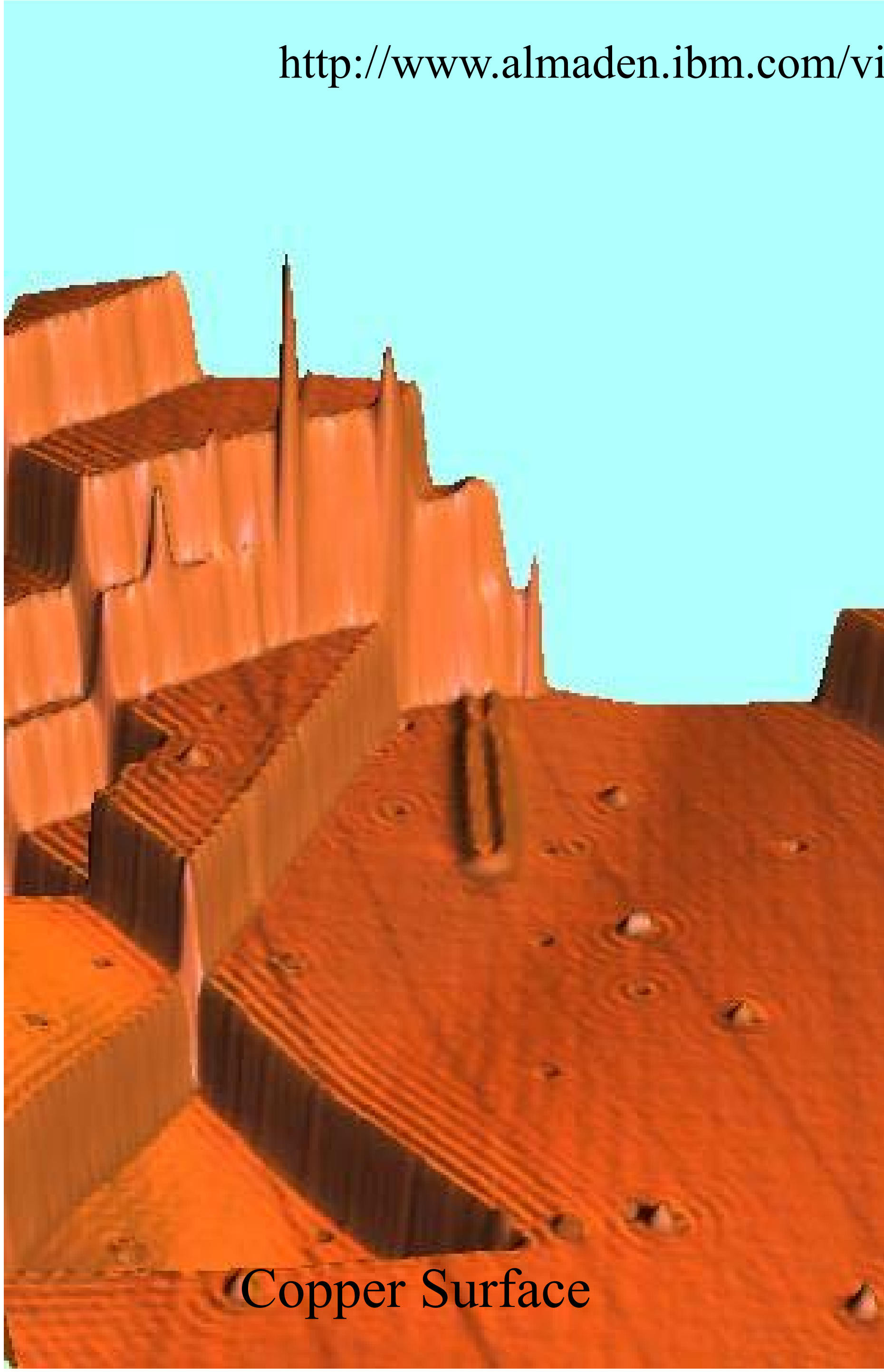
Only wave vectors $k < k_F$ can contribute to the screening

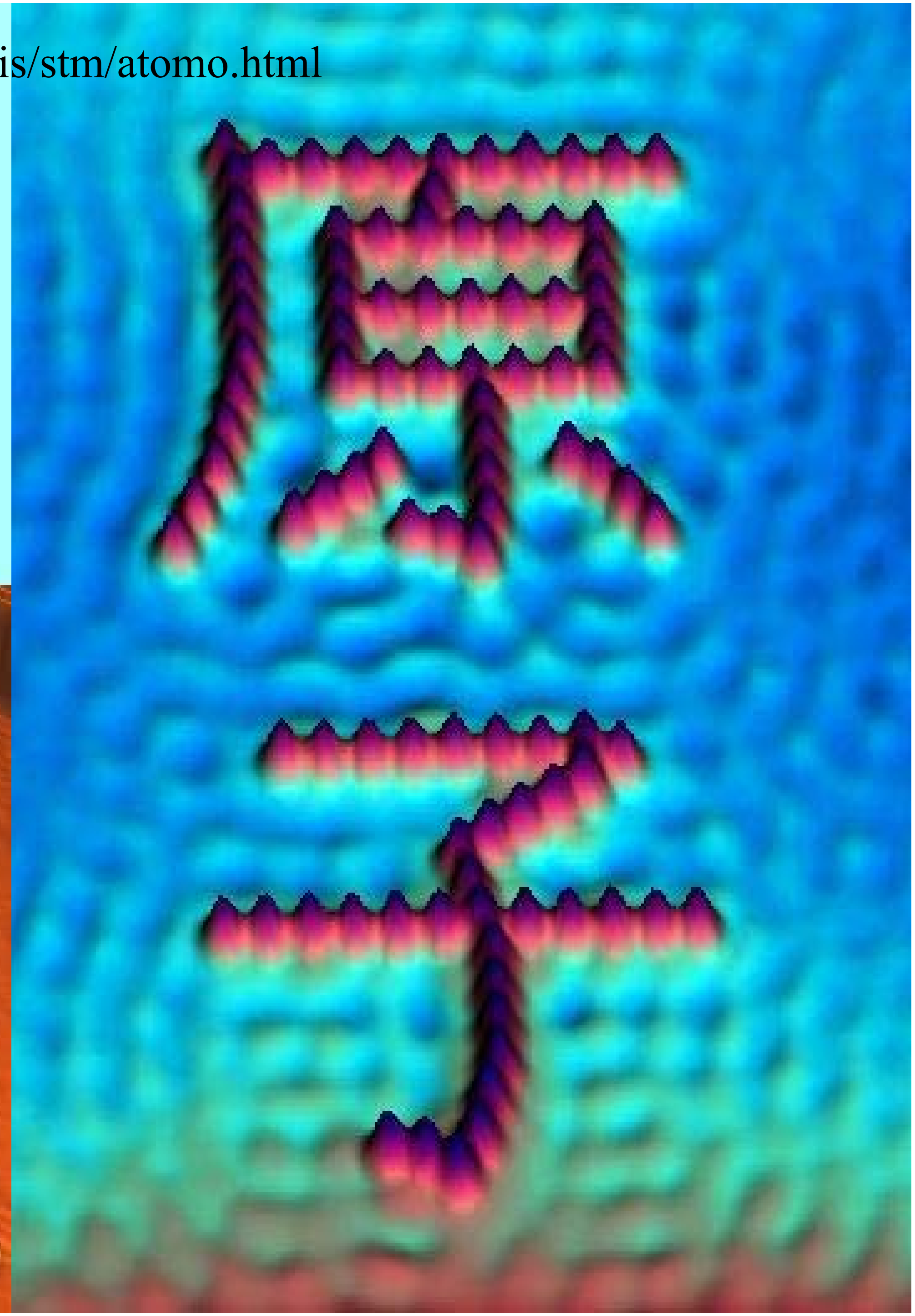


Around a point defect $$\frac{\sin(k_F r)}{r}$$



Friedel oscillations or Rudermann-Kittel oscillations http://www.almaden.ibm.com/vis/stm/atomo.html





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Direct Observation of Friedel Oscillations around Incorporated Si_{Ga} Dopants in GaAs by Low-Temperature Scanning Tunneling Microscopy

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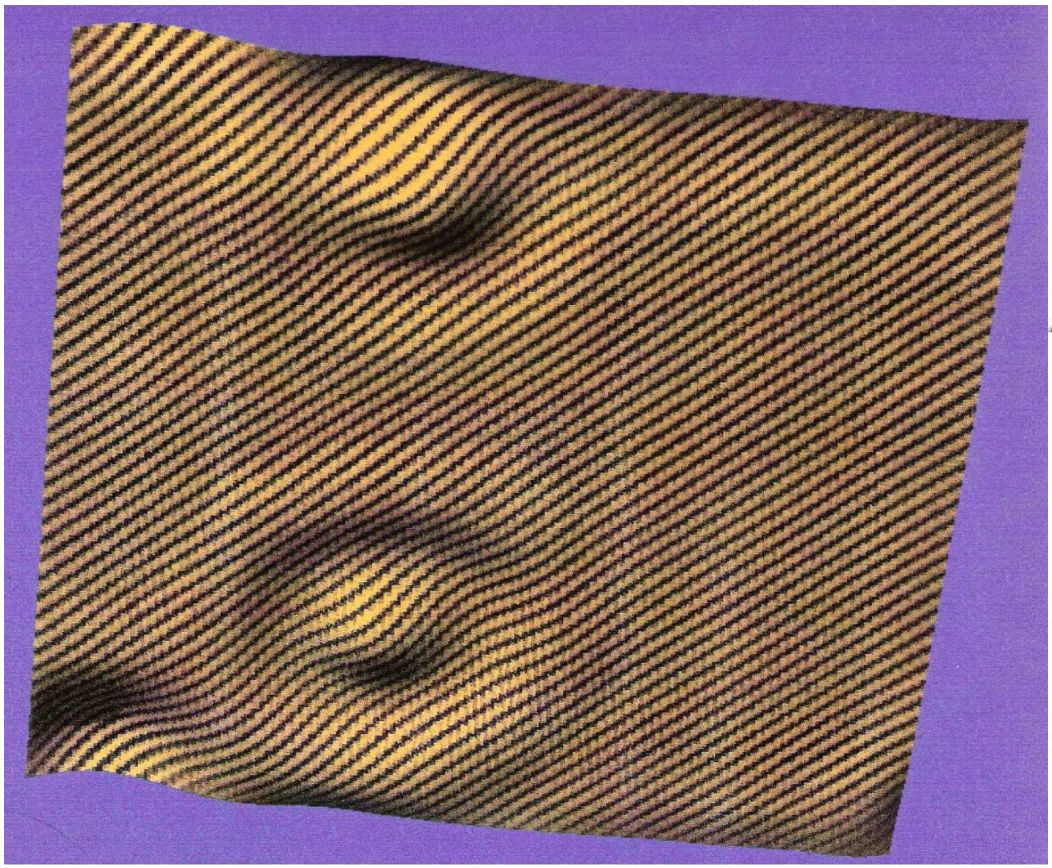
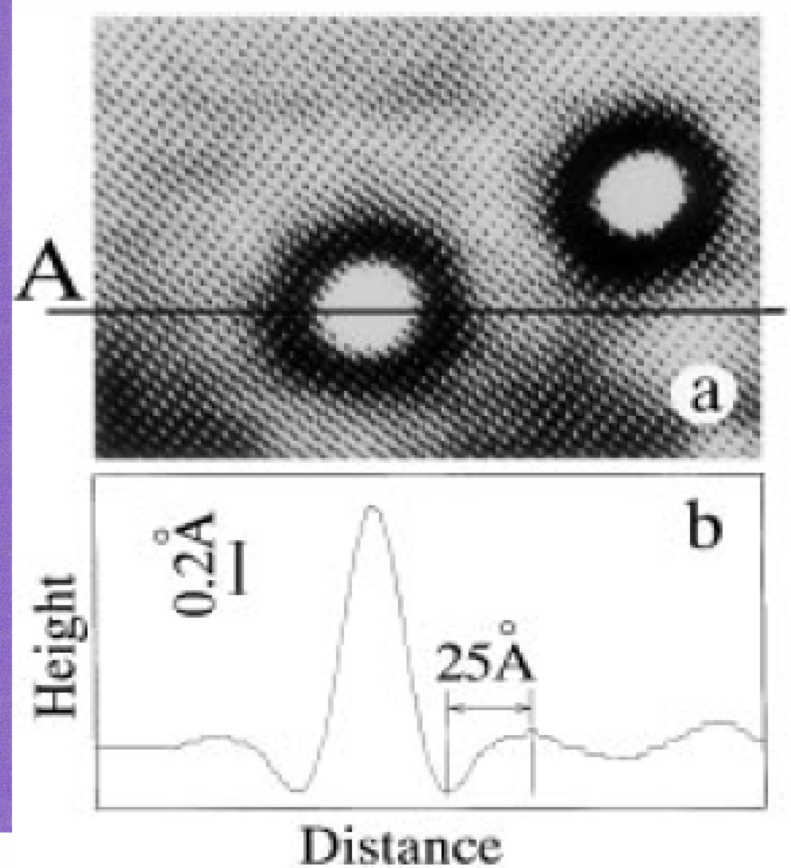
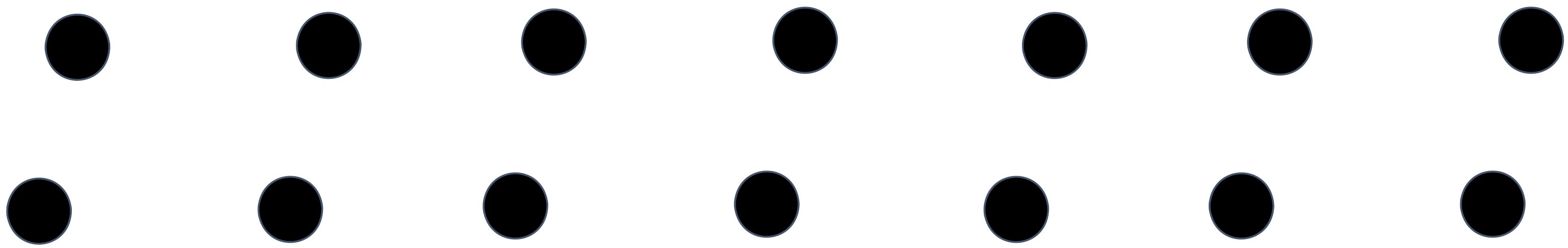
(Received 25 July 1995)

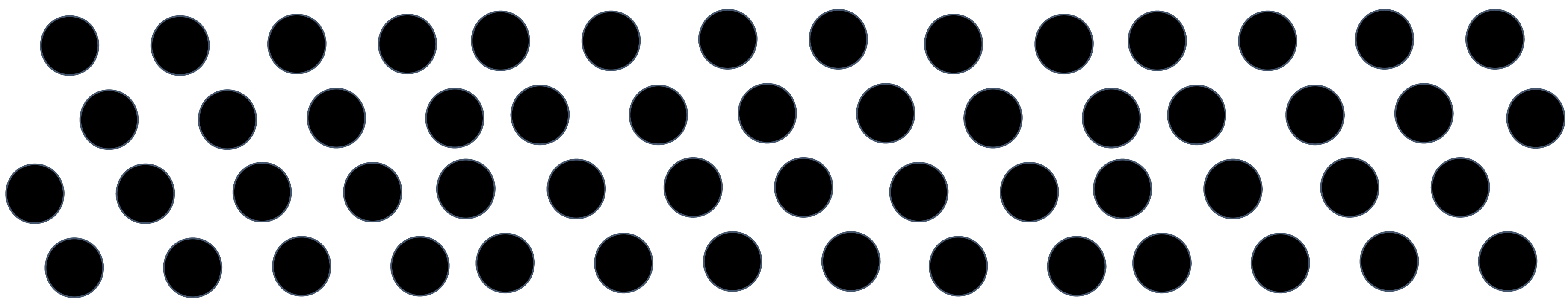




Metal-insulator transition

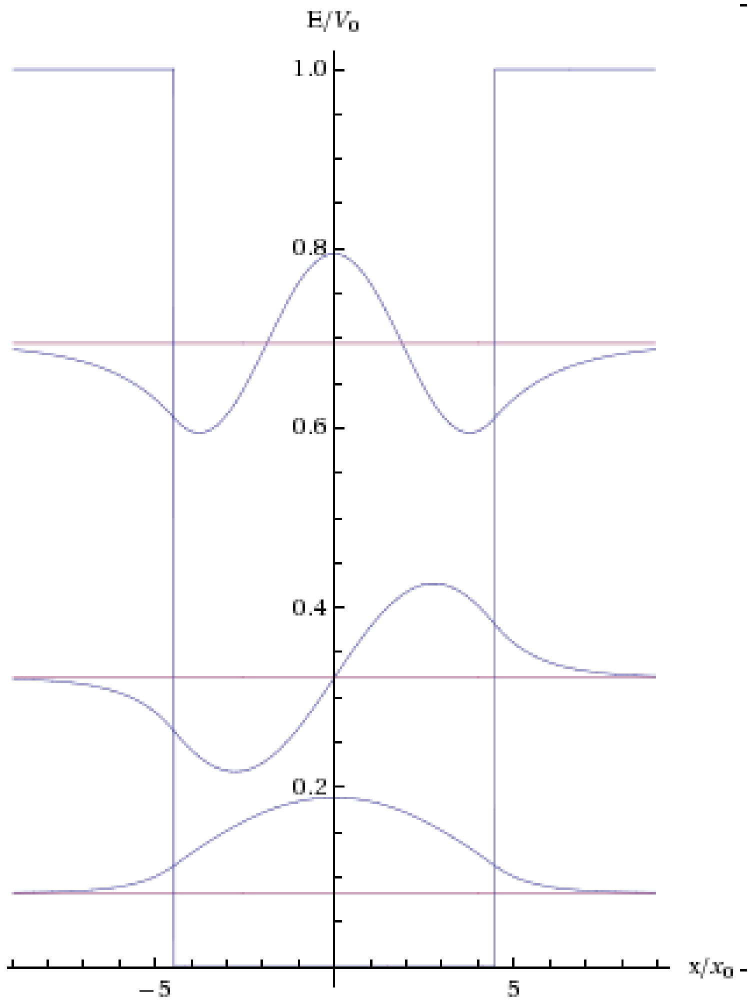


Atoms far apart: insulator



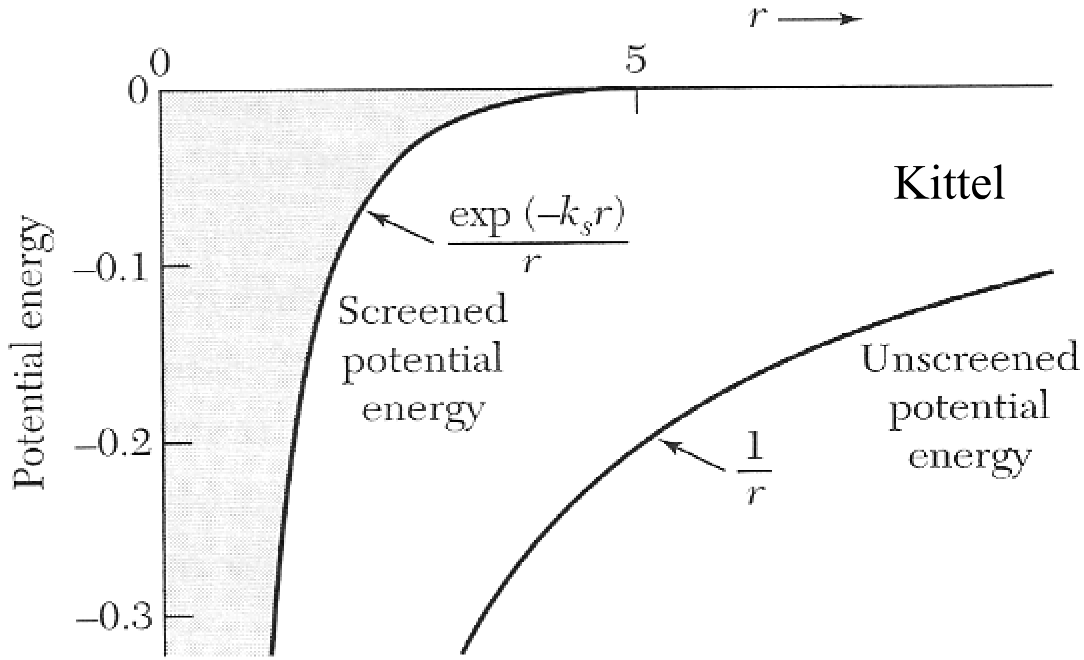
Atoms close together: metal

Mott transition



The number of bound states in a finite potential well depends on the width of the well. There is a critical width below which the valence electrons are no longer bound.

Mott transition

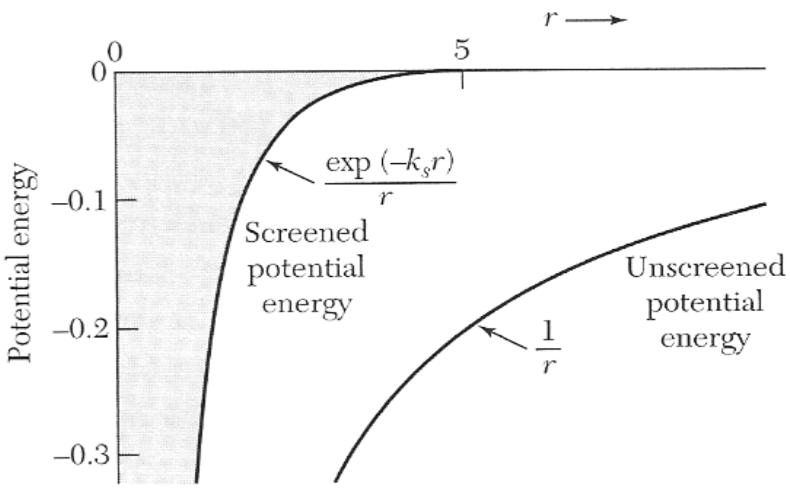


For low electron densities the screening is weak. The electrons are bound and the material is an insulator.

For high electron densities the screening is strong, the valence electrons are not bound and the material is a metal. The 1s state of a screened Coulomb potential becomes unbound at $k_s = 1.19/a_0$.

Mott transition (low electron density)

There are bound state solutions to the unscreened potential (hydrogen atom)



The 1s state of a screened Coulomb potential becomes unbound at $k_s = 1.19/a_0$.

Bohr radius

Nevill Francis Mott
Nobel prize 1977

Mott argued that the transition should be sharp.

$$k_s^2 = \frac{4}{a_0}\left(\frac{3n}{\pi}\right)^{1/3}$$

High-temperature oxide superconductors / antiferromagnets