Lecture 3: Electron spectroscopy - Photoemission & Co.

<table>
<thead>
<tr>
<th>Date</th>
<th>Topic</th>
<th>Guest</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monday 01/09</td>
<td>Golden / Goedkoop big introduction &amp; beginning of optical probes</td>
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<tr>
<td>Thursday 04/09</td>
<td>Golden / Goedkoop optical probes and inelastic electron scattering</td>
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<tr>
<td>Monday 08/09</td>
<td>Golden / Goedkoop photoemission and related probes</td>
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<tr>
<td>Thursday 11/09</td>
<td>Golden / Goedkoop x-ray spectroscopies</td>
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<tr>
<td>Friday 12/09</td>
<td>lab experiments</td>
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<tr>
<td>Monday 15/09</td>
<td>Borgschulte scanning tunneling microscopy / spectroscopy</td>
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<tr>
<td>Thursday 18/09</td>
<td>overspill: spectroscopy</td>
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<tr>
<td>Friday 19/09</td>
<td>lab experiments</td>
<td></td>
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<tr>
<td>Monday 22/09</td>
<td>you guys! preparing presentations: 'spectroscopy'</td>
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<tr>
<td>Thursday 25/09</td>
<td>all of us student presentations: 'spectroscopy'</td>
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<td>Friday 26/09</td>
<td>lab experiments</td>
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<tr>
<td>Monday 29/09</td>
<td>Eiser introduction light/x-ray scattering</td>
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<td>Thursday 02/10</td>
<td>Lohstroh thin film x-ray reflectivity / diffraction</td>
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<td>Friday 03/10</td>
<td>lab experiments</td>
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<td>Monday 06/10</td>
<td>Brück (3D) crystal structures from x-ray diffraction</td>
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<td>Thursday 09/10</td>
<td>Eiser structure in disordered systems &amp; soft matter</td>
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<td>Friday 10/10</td>
<td>lab experiments</td>
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<td>Monday 13/10</td>
<td>Wegdam dynamic light scattering and coherent x-rays I</td>
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<td>Thursday 16/10</td>
<td>Wegdam dynamic light scattering and coherent x-rays II</td>
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<td>Friday 17/10</td>
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<td>Monday 20/10</td>
<td>you guys preparing presentations: 'scattering'</td>
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<tr>
<td>Thursday 27/10</td>
<td>all of us student presentations: 'scattering'</td>
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</table>
### Lecture 3: Electron spectroscopy - Photoemission & Co.

#### EXPERIMENTS - spectroscopy:

<table>
<thead>
<tr>
<th>Date</th>
<th>Group</th>
<th>Exp.</th>
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<tbody>
<tr>
<td>5/9</td>
<td>3</td>
<td>optical absorption (WZI)</td>
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<td>electron spec. (WZI)</td>
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<td>2</td>
<td>STM (VU)</td>
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<td>19/9</td>
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<td>STM (VU)</td>
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<td></td>
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#### EXPERIMENTS - scattering:

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<tbody>
<tr>
<td>3/10</td>
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<td>DLS (WZI)</td>
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<td>2</td>
<td>thin film (VU)</td>
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<td></td>
<td>3</td>
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</table>
Research papers:

these will be distributed
today (as part of a break)

Lecture 3: Electron spectroscopy - Photoemission & Co.

first 30 minutes
i) dealing with the questions from last lecture(s)
ii) mini-report from the optical absorbers

hour #1 - photoemission: theoretical background
1) simple overview, including rough guide: 'how to do it'
2) Auger electron spectroscopy
3) PES of valence bands
4) PES of core levels
5) resonant photoemission
6) angle-resolved photoemission

hour #2 - photoemission: examples (ca. matching 2-6 above)
Photoelectron spectroscopy
or
photoemission

Some types of spectroscopy

<table>
<thead>
<tr>
<th>Probing particles</th>
<th>Method</th>
<th>Information about</th>
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</thead>
<tbody>
<tr>
<td>Photon in, electron out</td>
<td>PES</td>
<td>occupied states</td>
</tr>
<tr>
<td>Electron in, photon out</td>
<td>IPES</td>
<td>unoccupied states</td>
</tr>
<tr>
<td>Photon in, photon out</td>
<td>XES, RIXS, reflectivity, ellipsometry</td>
<td>occupied states, conduction electron dynamics</td>
</tr>
<tr>
<td>Photon in</td>
<td>XAS, absorption</td>
<td>unoccupied states, band gap, defect states</td>
</tr>
<tr>
<td>Electron in, electron out</td>
<td>EELS</td>
<td>collective excitations</td>
</tr>
<tr>
<td>Electron in or electron out</td>
<td>STM / STS</td>
<td>occupied or unoccupied states (local)</td>
</tr>
</tbody>
</table>
Spectroscopies with electrons

PES  XPS  IPES  XAS  AES  EELS

N-1  N-1

N+1  N, can be

N+1  N-2

N

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The Electromagnetic Spectrum

pic: courtesy of ALS

today
What can we learn using PES?

- atomic composition of a solid (surface)
- identity, structure, bonding and electronic structure of adsorbates and surface layers
- depth / spatial distribution of chemical species
- valence (conduction) band density of states
- valence (conduction) band structure $[E(k,\omega)]$
  - band widths / effective masses / Fermi surfaces
  - energy splittings/gaps - crystal field, exchange, superconducting interactions - self energies / lifetimes
- chemical-state/spin resolved spatial info. - microscopy
Pedestrian guide to PES

- conceptually very simple

\[ KE = h\nu - BE \]

- binding energy of the electron in the crystal

- kinetic energy of photoelectron in the vacuum

- experimental beginnings:
  - Heinrich Hertz at end of 19th century

- theoretical beginnings:
  - Albert Einstein at beginning of 20th century (→ Nobel prize)

Three step model for PES

- simple

- purely phenomenolgical, but useful

- step 1
  - incoming photon causes an optical transition in the solid
  - \( 'vertical' \) transition
Three step model for PES

- simple
- purely phenomenolgical, but useful

- step 2
  transmission of the photoelectron through the solid (towards surface)
  - energy-loss processes
  - secondary electrons
  - inelastic mean free path, $\lambda$

- step 3
  transmission of the photoelectron across the surface and into the vacuum
  - through surface potential barrier
  - $k_\perp$ not conserved
3 step model

(1) photoexcitation

(2) transport to surface

(3) transmission across surface

Energy

$E_v$  $hv$

$E_F$

sample  vacuum

Secondary electron cut-off

Generic spectrum

e.g. VB of gold

$E_F$

$hv - \Phi_{sample}$

$hv - \Phi$

Binding energy  0

Kinetic energy  $hv - \Phi$
**Lecture 3: Electron spectroscopy - Photoemission & Co.**

**'Fermi edge'**
- PES is ionising spectroscopy
- In metals: direct measure of Fermi-Dirac distribution:
  \[
  \frac{1}{e^{\frac{E-E_F}{k_BT}} + 1}
  \]
- If \( T_{\text{sample}} \) low enough, the 10%-90% width of the Fermi edge (≈FWHM Gaussian) measures the experimental energy resolution.

**Surface sensitivity**
- Cross section for inelastic scattering of photoelectrons during steps 2,3 is HIGH!

**notes:**
- \( 3\lambda = 3 \text{ nm} \)
- A few atomic layers!

\[ KE_{\text{e,vacuum}} = h\nu - BE_{\text{e,crystal}} \]
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**IMFP**
- inelastic mean free pathlength, \( \lambda \)
- \( \lambda \) defined as path length after which transmitted signal = \( 1/e \) of original signal

scattering cross-section for electron-electron scattering:

\[
\frac{d^2 \sigma}{d\Omega dE} = \frac{1}{(\pi a_0)^2} \cdot \frac{1}{q^2} \cdot \text{Im} \left\{ -\frac{1}{\epsilon(q, \omega)} \right\}
\]

loss function: just like in EELS

---

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**IMFP**
- inelastic mean free pathlength, \( \lambda \)

- for \( KE > 10 \) eV, all substances 'look' alike to a photoelectron: all resemble a free electron gas

- plasmon energy proportional to electron density (mean e-e distance)

\[
\omega_p = \sqrt{\frac{ne^2}{\epsilon_0 m}}
\]

- inverse average escape depth, \( \lambda^{-1} \):

\[
\sqrt{3} \frac{a_0 R}{KE} r_s^{-3/2} \ln \left( \frac{4}{9\pi} \right)^{2/3} \frac{KE}{R} r_s^2
\]

\( a_0 = \) Bohr radius, \( R=13.6 \) eV, \( r_s \): mean e-e distance (in \( a_0 \)'s)
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IMFP

'universal' curve

\[ \lambda (\text{Å}) \]

\[ KE (\text{eV}) \]

- \( \lambda \) does depend on material: e.g. metal or ionic insulator etc. (particularly for low KE)
- \( \lambda = \text{small} \) small !! surface sensitivity

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**surface preparation**

as $\lambda$ is so small, in order not to do research into dirt, the surface of the system has to be prepared to be clean.....

- annealing
- sputtering & annealing
- cleavage
- filing

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**keeping** the surface clean

air (1 bar)

$1$ microsecond later.... $\left(10^{-6} \text{ s}\right)$

- signal contaminated
- surface modified
keep clean via ....  

* ultra high vacuum *

pumping

\[ \text{10}^{-11} \text{ mbar} = \text{10}^{-14} \text{ bar} = \text{UHV} = \text{10}^5 \text{ seconds (27 hours) for experiments} \]

---

Ultra high vacuum \( = 0.0000000000001 \text{ atm.} \)

- CF-flange system (knife edges + copper gaskets)
- stainless steel chambers, valves, CF components
- pumps: turbomolecular pumps, ion pumps (+NEG), titanium sublimation pumps, cryopumps
- desorb water molecules that are 'stuck' to the internal surfaces via a 'bakeout' at 180-200°C
- all materials: strong + low vapour pressure (also @ 200°C)

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**Light sources**
- VUV photons
- X-ray photons

**In the lab**
- Synchrotron radiation

**Synchrotron radiation**
- Intense, brilliant
- Selectable energy = monochromatic
- Selectable polarisation

- VUV: too high E for lasers
- No windows possible
- Reflecting optics
Analysis of photoelectrons

- kinetic energy
- emission angle w.r.t. surface normal

2D detector:
- axis no. 1 = KE
- axis no. 2 = \( \theta \)
- 2D data cut into slices parallel to either of the two axes

Pic: Damascelli

Resolution in 1990:
- \( E: 30-80 \text{ meV} \)
- \( \Delta \theta: 2^\circ \)

Resolution in 2000:
- \( E: 10-30 \text{ meV} \)
- \( \Delta \theta: 0.3-0.6^\circ \)

Resolution in 2003:
- \( E: < 1.5 \text{ meV} \)
- \( \Delta \theta: 0.1-0.3^\circ \)

Resolution in 2006?
- \( E: 0.1 \text{ meV} \)
- \( \Delta \theta: 0.1^\circ \)
- \( T_{\text{crystal}}: 300 \text{ mK} \)

What do we need?
- \( 4k_B T (10K) = 3.2 \text{ meV} \)
- \( \Delta k = 0.5\% \pi/a = 0.1^\circ \)
Fermi’s golden rule

transition probability:

energy conservation

\[ w_{ji} = \frac{2\pi}{\hbar} |\langle \Psi_f^N | H_{\text{int}} | \Psi_i^N \rangle|^2 \delta(E_f^N - E_i^N - h\nu) \]

BE of photoelectron of KE=E_{\text{kin}} and momentum k

what is \( H_{\text{int}} \)?

\[ H_{\text{int}} = \frac{\epsilon}{2m\epsilon_c} (\mathbf{A} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{A}) = \frac{\epsilon}{m\epsilon_c} \mathbf{A} \cdot \mathbf{p} \]

What does PES intensity mean?

the story behind \( H_{\text{int}} \):

- terms quadratic in \( \mathbf{A} \) have been dropped
- use commutator relation: \( [p, A] = i\hbar \nabla \cdot A = 0 \)
- use dipole approximation: \( A \) constant on scale of atomic dimension, thus \( \nabla \cdot A = 0 \) OK for VUV and x-ray ranges
- beware! \( \nabla \cdot A = 0 \) may be poor approx. at the surface
- thus, step 1 is a dipolar optical excitation
Sudden approximation

- We'd like to factorise the wave-functions here into N-1 electron and photoelectron terms (like done for E):

\[
E_i^N = E_i^{N-1} - E_k^N \quad \text{and} \quad E_f^N = E_f^{N-1} + E_{\text{kin}}
\]

- This is highly non-trivial as the system will relax during photoemission

- Sudden approximation: electron instantaneously removed and discontinuous change in effective potential for system

- OK for high kinetic energies: e.g. 20eV is enough in HTSC

Factorise final state wave-function:

\[
\Psi_f^N = A \phi_f^k \Psi_f^{N-1}
\]

- \(A\) antisymmetrises the N-electron wavefunction so Pauli principle is obeyed

\(\phi_f^k\) is the wavefunction of the photoelectron with \(k\)

\(\Psi_f^{N-1}\) is the final state wavefunction of the (N-1)-electron system left behind

- Chosen as excited state with eigenfunction \(\Psi_m^{N-1}\) and energy \(E_m^{N-1}\)

- Total transition probability: sum over all possible \(m\)
Sudden approximation

- Factorise initial state wave-function:

\[ \Psi_i^N = A \phi_i^k \Psi_i^{N-1} \]

single Slater determinant (HF)

- Not an eigenstate of the (N-1) particle Hamiltonian!

- \( \Psi_i^{N-1} = c_k \Psi_i^N \)

- Better

- \( c_k \) annihilates an electron with momentum \( k \)

Sudden approximation

- Matrix elements now:

\[ w_{fi} = \frac{2\pi}{\hbar} |\langle \Psi_f^N | H_{int} | \Psi_i^N \rangle|^2 \delta(E_f^N - E_i^N - h\nu) \]

- Rename:

\[ M_{f,i}^k = \langle \phi_f^k | H_{int} | \phi_i^k \rangle \]

one-electron dipole matrix element

(N-1)-electron overlap integral
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**Total intensity**

- Total intensity
  \[ I(k, E_{\text{kin}}) = \sum f_{i} w_{f,i} \]

- Thus, total intensity =
  \[ \sum_{f_{i}} |M_{f,i}^{k}|^{2} \sum_{m} |c_{m,i}|^{2} \delta(E_{\text{kin}} + E_{m}^{N-1} - E_{i}^{N} - h\nu) \]

for \( E = E_{\text{kin}} \) and momentum = \( k \)

\[ |c_{m,i}|^{2} = |\langle \Psi_{m}^{N-1} | \Psi_{i}^{N-1} \rangle |^{2} \]

probability that on removing an electron from state \( i \), the \((N-1)\)-electron system is left in excited state \( m \)

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**Selection rules**

- \( M_{f,i}^{k} \equiv \langle \phi_{f}^{k} | H_{\text{int}} | \phi_{i}^{k} \rangle \)

- \( |M_{f,i}^{k}|^{2} \) non-zero for:
  \[ \Delta l = \pm 1 \]
  \[ \Delta m = +1, 0, -1 \]

\[ s \rightarrow p \]
\[ p \rightarrow s,d \]
\[ d \rightarrow p,f \]
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Selection rules

- if $\Psi_i^{N-1} = \Psi_{m0}^{N-1}$ for $m = m_0$
- then $|c_{m_0,i}|^2 = 1$, and all other $c_{m,i} = 0$
- in this case, if $M_{f,i}^k \neq 0$

- PES spectrum is a delta function at HF orbital energy $E_D^k = -\epsilon_k$

Koopman's theorem

Other excitations

- in reality, many $|c_{m_0,i}|^2$ are non-zero
- then, spectrum = main line satellites

PES spectrum of $H_2$ molecule

Pics: Damascelli
One particle spectral function

- in reality, many $|c_{T(\omega)}|^2$ are non-zero
- Green's function approach is a good one

\[
G^\pm(k, \omega) = \sum_m \frac{|\langle \Psi_m^\pm | c_k^\dagger | \Psi_1^\mp \rangle|^2}{\omega - E_m^\pm + i\eta}
\]

for electron addition or removal

- obtain one particle spectral function:

\[
A(k, \omega) = A^+(k, \omega) + A^-(k, \omega) = -(1/\pi) \text{Im} G(k, \omega)
\]

\[
A^\pm(k, \omega) = \sum_m |\langle \Psi_m^\pm | c_k^\dagger | \Psi_1^\mp \rangle|^2 \delta(\omega - E_m^\pm + E_i^N)
\]

photoemission = $A^-(k, \omega)$

inverse photoemission = $A^+(k, \omega)$

\[
I(k, \omega) = I_0(k, \nu, A) f(\omega) A(k, \omega)
\]
**Measured quantity in (AR)PES**

\[ I(k, \omega) = I_0(k, \nu, A) f(\omega) A(k, \omega) \]

- contains effects of Fermi distribution spectral function
- *plus* extrinsic background
- *plus* finite energy and momentum resolution

**Self energy**

- correction to Green's functions from e.g. electron correlations:
  \[ \Sigma(k, \omega) = \Sigma'(k, \omega) + i\Sigma''(k, \omega) \]
  - electron proper self-energy
  - energy renormalisation
  - lifetime

- in many body, interacting system
Self energy and the spectral function

- Green's function:
  \[ G(k, \omega) = \frac{1}{\omega - \varepsilon_k - \Sigma(k, \omega)} \]

- Spectral function:
  \[ A(k, \omega) = -\frac{1}{\pi} \frac{\Sigma''(k, \omega)}{[\omega - \varepsilon_k - \Sigma'(k, \omega)]^2 + [\Sigma''(k, \omega)]^2} \]

Fermi liquid spectral function

- Green's function:
  \[ G(k, \omega) = \frac{Z_k}{\omega - \varepsilon_k + i\Gamma_k} + G_{\text{incoh}} \]

- Spectral function:
  \[ A(k, \omega) = \frac{\Gamma_k}{(\omega - \varepsilon_k)^2 + \Gamma_k^2} - A_{\text{incoh}} \]

- QP's:
  \[ \varepsilon_k = \frac{m^*}{\hbar^2} \]
  \[ \tau_k = \frac{2\hbar}{\Gamma_k} \]
Fermi liquid spectral function

Spectral function:

\[ A(k, \omega) = Z_k \frac{\Gamma_k/\varepsilon}{(\omega - \varepsilon_k)^2 + \Gamma_k^2} + A_{\text{inc}} \]

Condition: \( \varepsilon_k - \mu \gg |\Sigma''| \) for small BE and near \( k_F \)

Consequence:

\[ \Gamma_k \propto \left[ (\pi k_B T)^2 + (\varepsilon_k - \mu)^2 \right] \]

Width of QP feature = quadratic in BE / or T (depending which is greater)

Lifetimes contd.

Energy widths in PES are dominated by hole lifetime:

\[ \tau_h^k = \frac{2\hbar}{\Gamma_h^k} \]

- \( \tau_h \ll \tau_e \)
- \( \tau_h \) are of the order of \( 10^{-15} \) seconds
- PES is a FAST probe
### Photoionisation cross sections

- **good match of initial and final state wavefunctions**

\[ M_{f,i}^k = \langle \phi_f^k | H_{\text{int}} | \phi_i^k \rangle \]

- **radial part of the wavefunction important**

**final state**! (selected via choice of \( h \nu \))

**optimal overlap:**
- low \( E_{\text{final}} \) + extended \( |i> \) (e.g. C 2s, 2p)
- high \( E_{\text{final}} \) + compact \( |i> \) (e.g. C1s)

\( \rightarrow \) use to discriminate between different \( |i> \)

### Core level photoemission "XPS"

- **x-ray photoelectron spectroscopy**

- core levels strongly localised, thus BE's give elemental identification

- chemical shifts give information on:
  - chemical environment of emitter
  - oxidation / valence / bonding state

- **satellites and/or shake up** are the response of system to core ionisation

- **angular distribution** (PhD, XPD) is a local, non-destructive structural probe

\( \text{N-1} \)
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- XPS as ESCA ‘Electron Spectroscopy for Chemical Analysis’
- PES

Core level BE signals which element
- Exact BE can give info about chemical environment
- Surface sensitive chemical analysis
- C atoms in four different surroundings

Chemical shifts
- BE increases as more electronegative groups as partners or oxidation state is higher
  - e.g. Al metal has Al2p BE of 72.6 eV
  - Al₂O₃ 75.3 eV
- In fact, chemical shifts are the result of (partial) cancellation of two terms of order 10-20 eV (!!): a screening charge term and a Madelung term
  - Beware: they can lie !!
  - Screening in the final state also plays a crucial role
Shake up

- A same time as photoelectron is emitted, another elementary excitation is generated:
  - phonon
  - plasmon
  - interband transition
  - intraband (e-h) transitions

- Shake-up costs energy, thus $E_{\text{shake-up}} > E_{\text{main line}}$

  - In shake-up, not only dipole, but also monopole transitions are allowed

Resonant photoemission

- Photon energy tuned to a core-level threshold
Resonant photoemission

- these two final states interfere

- non radiative super-Coster-Kronig decay of the core hole

Resonant photoemission

- involvement of the core hole:
  
  - enhances cross section for valence emission from orbitals of the same atom whose core level is used
  
  - $\tau_h$ can be used as a 'core level clock'
Auger electron spectroscopy (AES)

- Routine surface analysis tool

Electrons as excitation source easier than photons as no high level of monochromaticity required

Angle-resolved core level photoemission (XPD, PhD)

- Outgoing photoelectron = spherical wave
- For higher KE, this can forward scatter from surrounding atoms

- Analyse core-level intensity vs. offtake angles $\theta, \phi$
- Analyse core-level intensity vs. $h\nu$
Angle-resolved photoemission (ARPES)

- single crystalline sample
- angle-resolved detection of photoelectrons

How to determine $k_{||}$

- $KE = \frac{1}{2}mv^2$, $p = mv$
  - $KE = \frac{1}{2}p^2/m$
  - $p = (2mKE)^{\frac{1}{2}}$

- momentum component parallel to surface, $p_{||}$
  \[ p_{||} = p \sin \theta = (2mKE)^{\frac{1}{2}} \sin \theta \]

- $k$ vector parallel to surface, $k_{||}$
  \[ k_{||} = \frac{p_{||} \hbar}{\hbar} = (2mKE / \hbar^2)^{\frac{1}{2}} \sin \theta \]

  \[ k_{||} = \sqrt{2mE_{\text{kin}}} \sin \theta \]

- vertical transitions and $k_{||}$-conservation across surface
ARPES

what about $k_i$?

\[ K_{\text{final}}^\perp = \sqrt{K_{\text{vac}}^\perp^2 + \frac{2m}{\hbar^2} V_0} \]

\[ K_{\text{vac}}^\perp = \frac{2m}{\hbar^2} E_{\text{kin}} \cdot \cos \theta \]

inner potential $V_0$

(w.r.t. bottom of band) electrons feel an attractive potential, $V_0 = E_F + \Phi$

ARPES for 2D systems

$k_i$ not important for the energy variation of the electronic states

\[ |k_i| = \frac{\sqrt{2mE_{\text{kin}}}}{\hbar} \sin \theta = 0.512 \sqrt{E_{\text{kin}}(eV)} \sin \theta \]

in Å\(^{-1}\) in eV in degrees
EXAMPLES

1) Auger electron spectroscopy
2) PES of valence bands
3) PES of core levels
4) resonant photoemission
5) angle-resolved photoemission

1st:
a fullerene reminder
Lecture 3: Electron spectroscopy - Photoemission & Co.

- truncated icosahedron
- $I_h$ symmetry

...the roundest molecule in the universe

Molecular solid

Non-polar: solid $C_{60}$ → FCC close packing

(111) surface
Close packed structures

FCC  HCP  BCC

pics: scottv@asu.edu

How can we alter the properties of C$_{60}$?

intercalation

interstitial sites


**LECTURE 3: ELECTRON SPECTROSCOPY**

**EXAMPLE 1**

1) Auger electron spectroscopy
**True 'transport' gap**

- $E_{N-1}$ electrons - $E_{N+1}$ electrons

- Optical transition is an 'on-ball' (Frenkel) exciton

- Exciton BE $\sim U = 1.5$ eV ??

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**AES of $C_{60}$**

- $C_{KVV}$ Auger and compare with self-convolution of the valence band PES

- $U$ is of order 1.5 eV!!
EXAMPLE 2

2) PES of valence bands

How can we alter the properties of C$_{60}$?

intercalation

interstitial sites
What should n-type intercalation do?

- partially fill the LUMO-derived conduction band
- \( t_{1u} \) - total six electrons

Satpathy et al., PRB, 1992

PES of CPES of \( C_60 \) and \( K_xC_60 \)

!! \( K_3C_{60} \) metallic, \( K_4C_{60} \) not
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PES of \( \text{C}_{60} \) - valence band PES of \( \text{C}_{60} \) and \( K_x \text{C}_{60} \)

core level shake-up also in valence band PES

Example 3

3) PES of core levels
Chemical shift gives structural information in $K_xC_{60}$.

Examples

4) resonant photoemission
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**Example 5**

5) angle-resolved photoemission
The nodal direction (0,0)-(\pi, \pi) as an illustration

A = antinode

N = node

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Energy Distribution Curves

Momentum Distribution Curves

State-of-the-art ARPES of a high Tc superconductor

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Binding energy (eV)

Momentum (Å⁻¹)

0.4 0.5 0.6 0.7
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**ARPES data - equal footing in either $E$ or $k$**

- **EDC - $I(k_x, k_y, E)$**
- **EDM - $I(k_x, k_y, E)$**

Borisenko et al., PRB 64, 094513 (2001)

**A full picture of $I_{PES}$ vs. the 3D $k_x, k_y, E_B$ space**

Borisenko et al., PRB 64, 094513 (2001)
Constant energy surfaces: E dependence

HTSC

300K, \( h\nu = 21 \text{ eV} \)

Kordyuk et al., 2000

That's it for this lecture.

Thursday: x-ray spectroscopies