

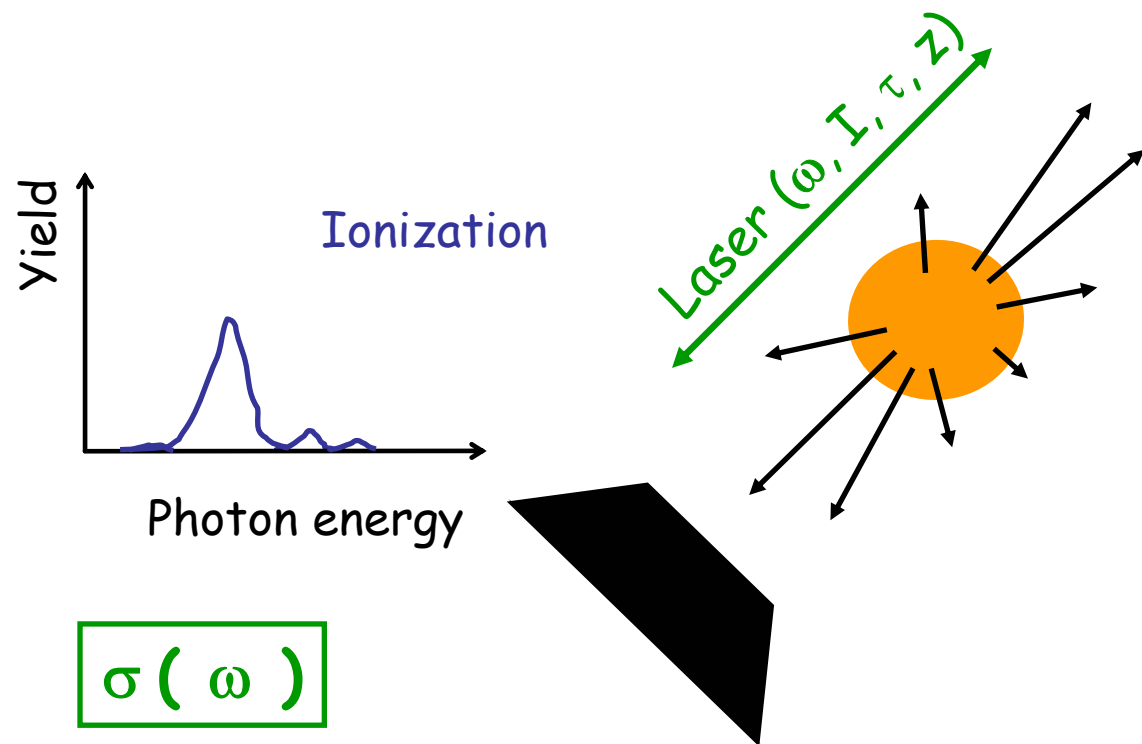
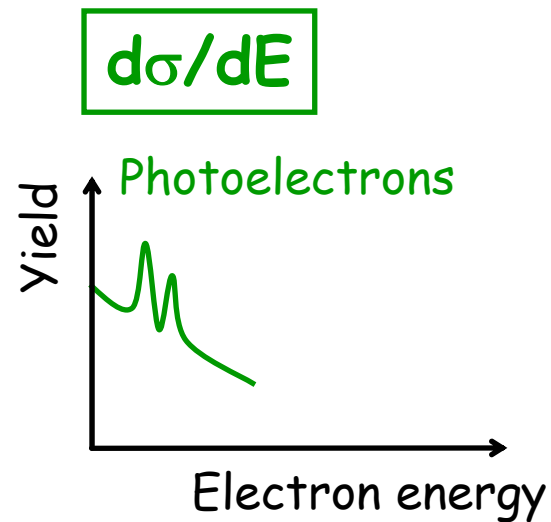
# Clusters in strong fields

## Correlations in electronic emission

- Electron emission from irradiated (free) metal clusters
- Kinetic energy spectra (Photo Electron Spectroscopy, PES)
- Angular distributions (Photoelectron Angular Distribution, PAD)
- Structure properties of clusters
- Dynamical properties (low/high ionization regimes)

# Electron emission from irradiated clusters

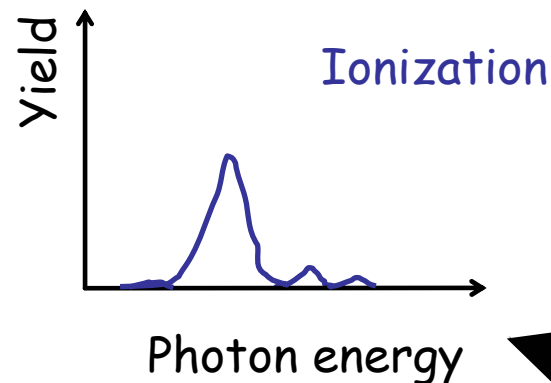
Optical laser - Moderate intensity



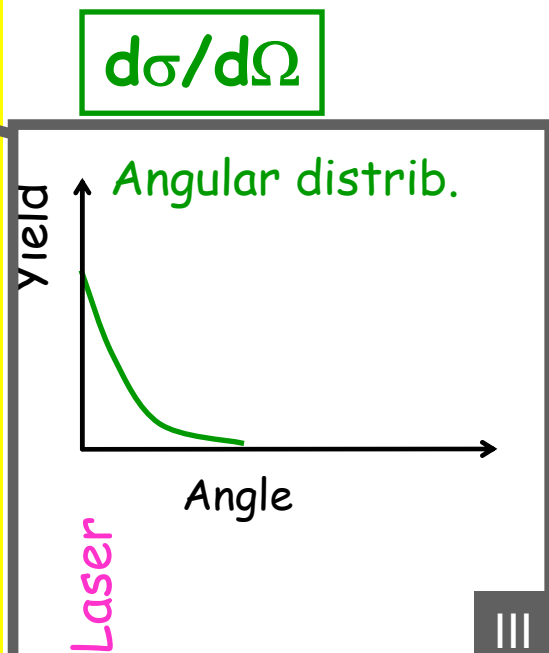
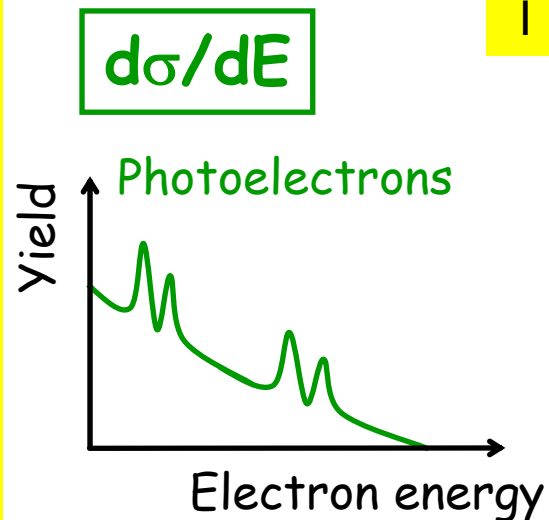
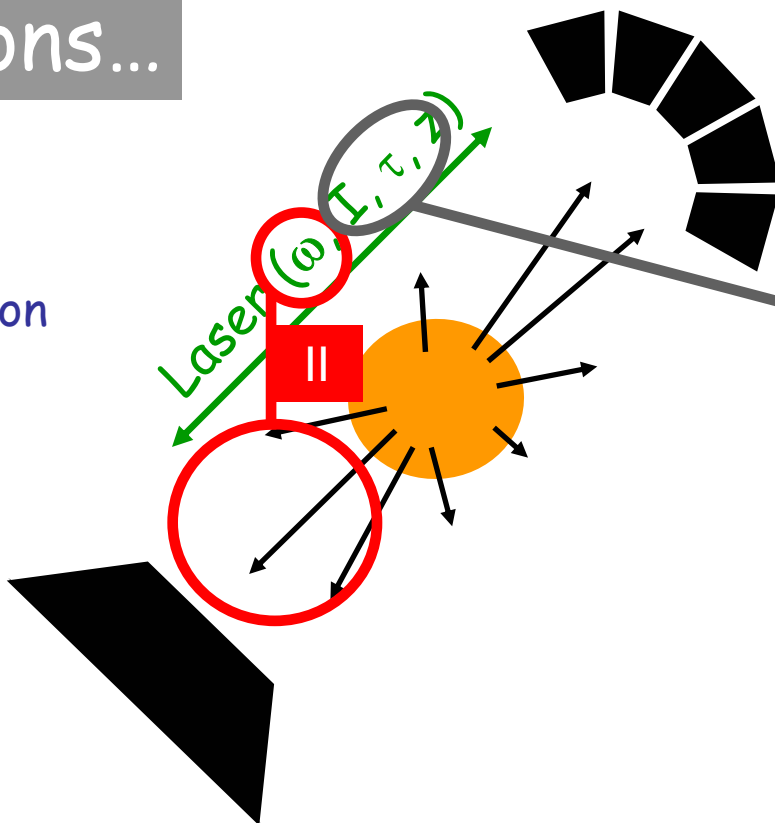
# Electron emission from irradiated clusters

Optical laser - Moderate intensity

Correlations...



$$\sigma(\omega)$$



# Which theory for which situations ?

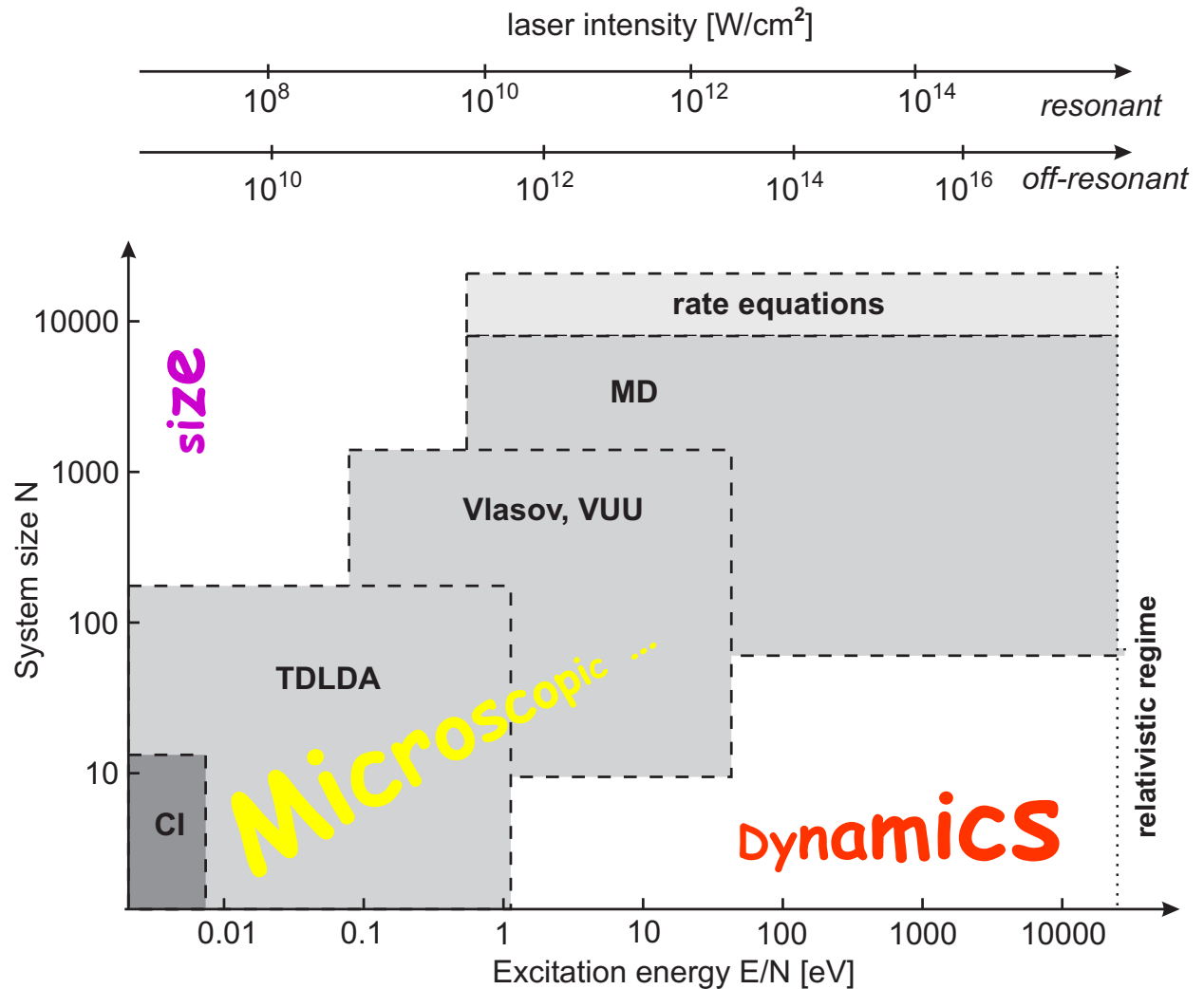
## Requirements

- Size
- Dynamics
- Microscopic ...



## Compromises

- No
- « final »
- Theory
- yet...
- Boundaries
- to explore ...



# TDLDA

➤ Electrons

- Time Dependent Density Functional Theory (TDDFT)

Ensemble of orbitals (1 electron) / no correlation  $\{\phi_i(\mathbf{r}), i = 1, \dots\}$

One body density

$$\rho(\mathbf{r}) = \sum_j |\phi_j(\mathbf{r})|^2$$

Effective mean field theory (Kohn-Sham)

$$i\hbar \frac{\partial \phi_i}{\partial t} = h[\rho] \phi_i$$

$$h[\rho] = -\frac{\hbar^2}{2m} \Delta + U_{\text{KS}} + U_{\text{ext}}(\mathbf{r}, t)$$

Kohn-Sham potential

Ions + ext.

- Local Density Approximation (LDA)

$$U_{\text{KS}} = U_{\text{H}} + U_{\text{xc}}[\rho]$$

Coulomb direct

Exch. + Corr.

+ Self Interaction Correction (SIC) ...

- Explicit ions via pseudo potentials

➤ Ions

- Detail of structure + ionic Molecular Dynamics (MD)

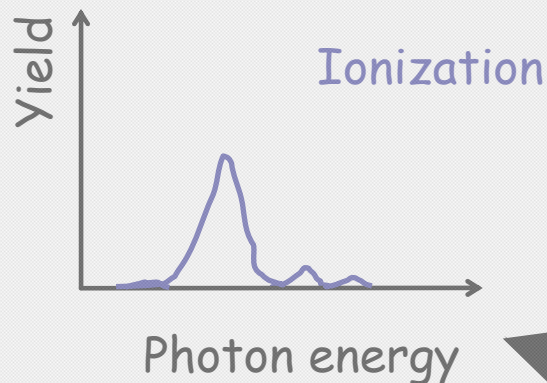


TDLDA-MD

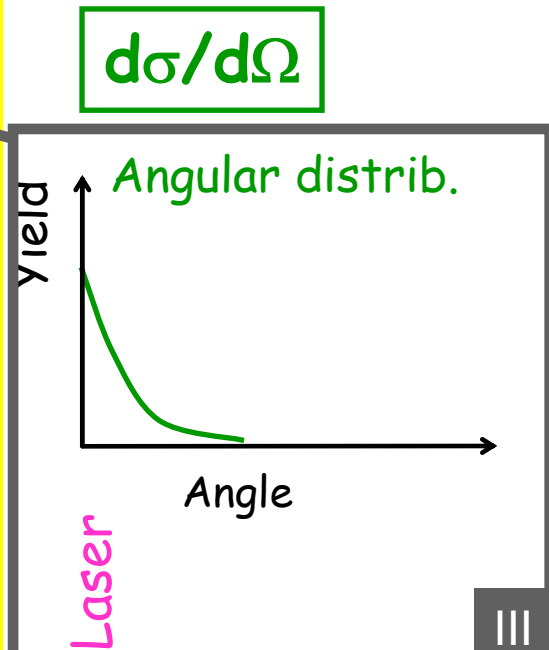
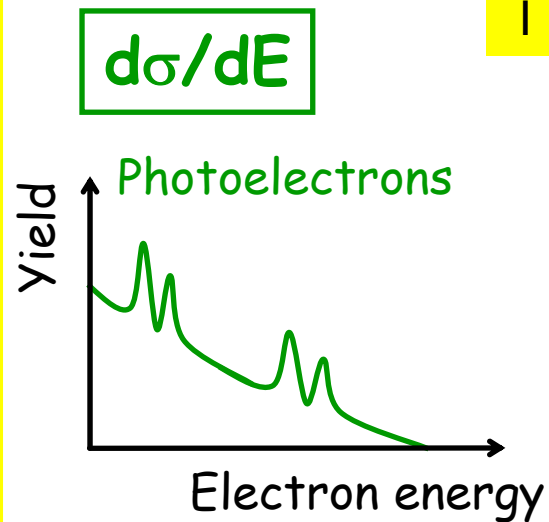
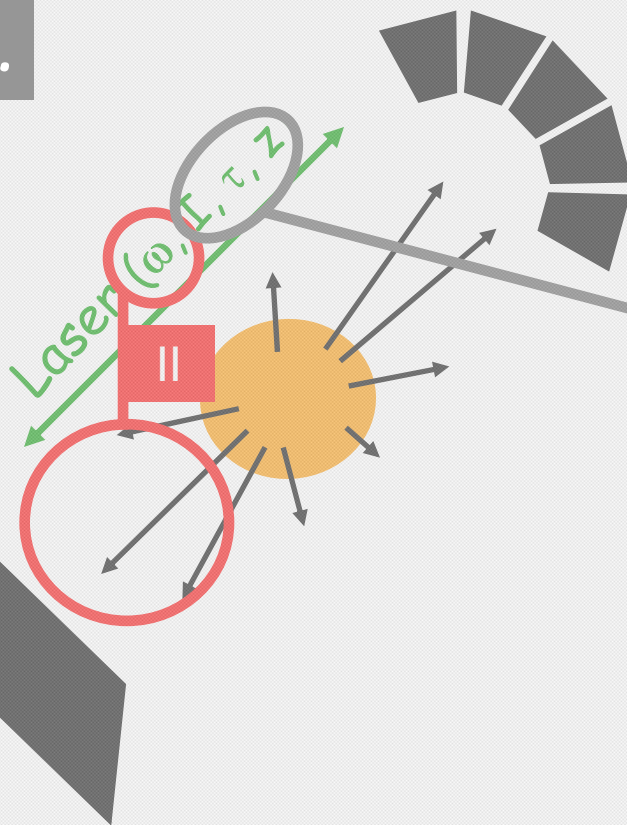
# Electron emission from irradiated clusters

Optical laser - Moderate intensity

Correlations...



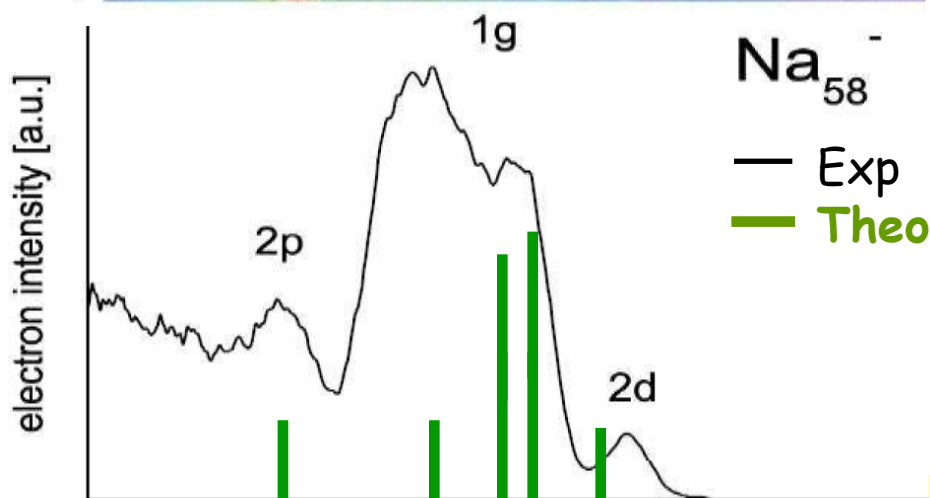
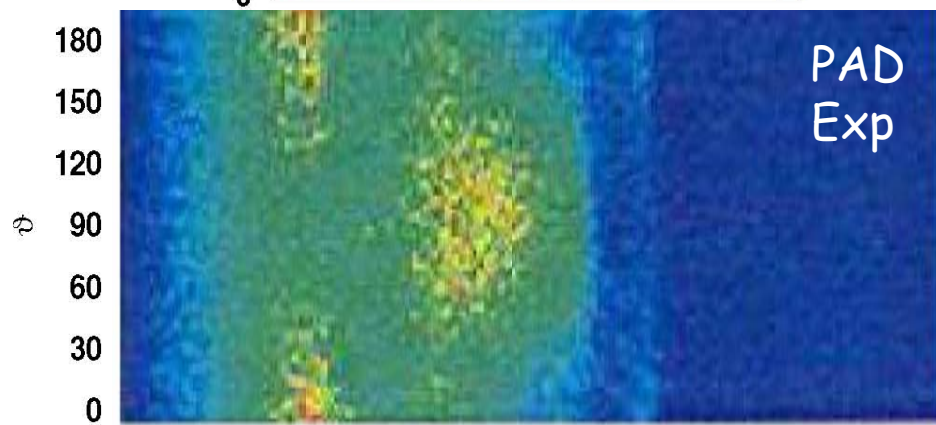
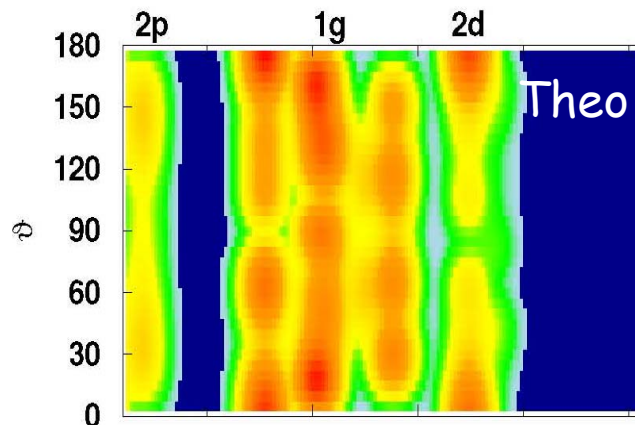
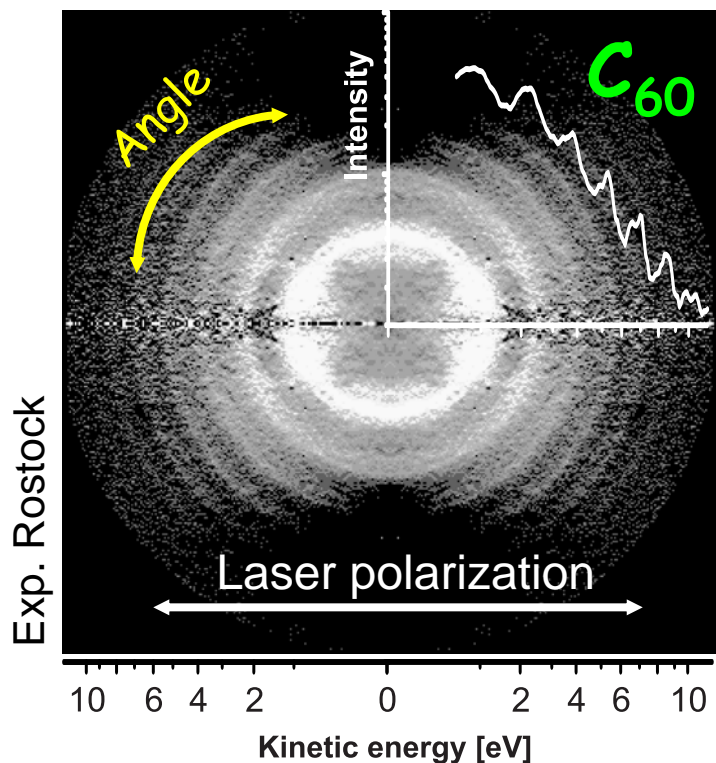
$$\sigma(\omega)$$



# Energy resolved angular distributions

Angle-energy correlation

→  $d\sigma/d\Omega dE$

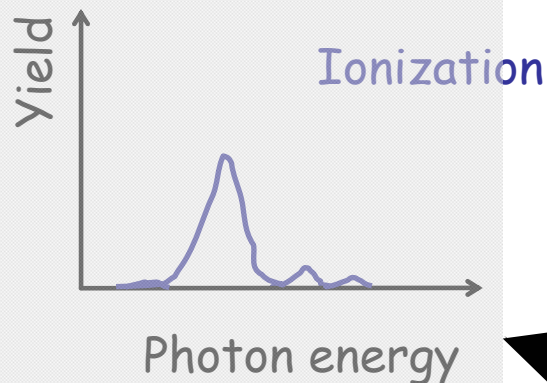




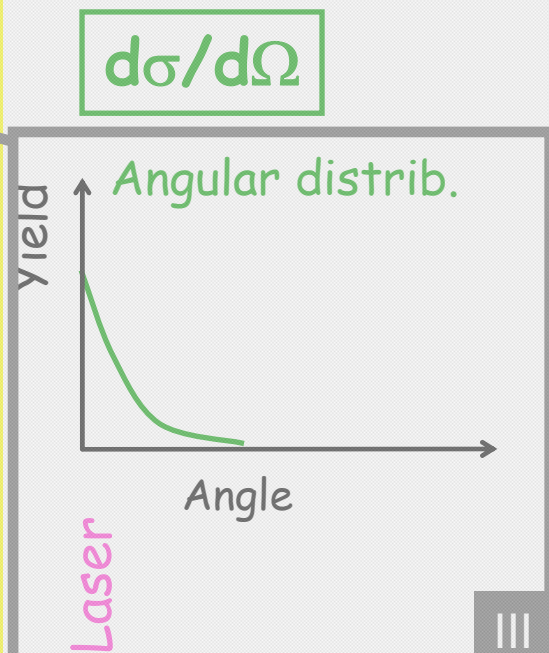
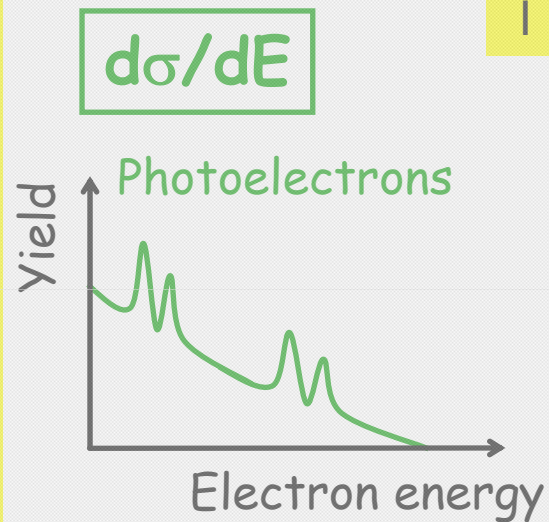
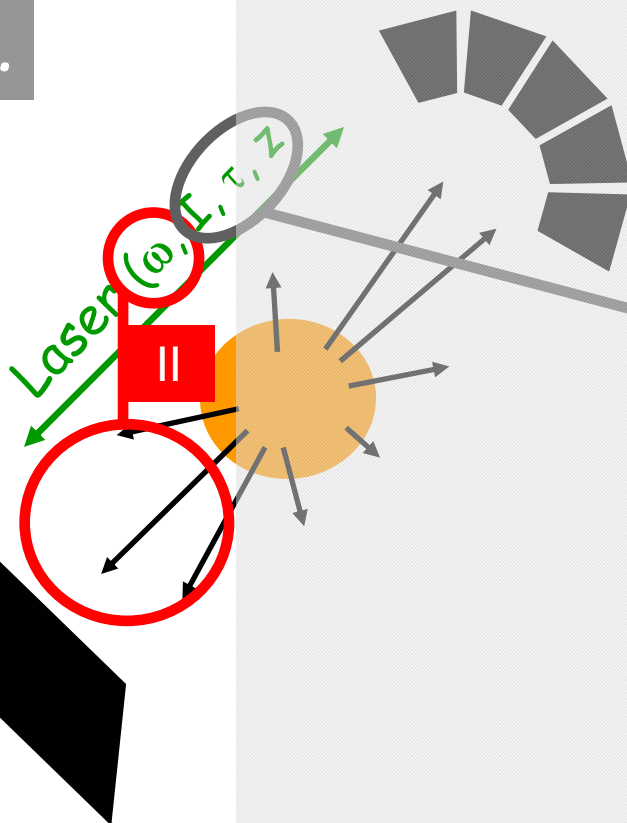
# Electron emission from irradiated clusters

Optical laser - Moderate intensity

Correlations...



$$\sigma(\omega)$$



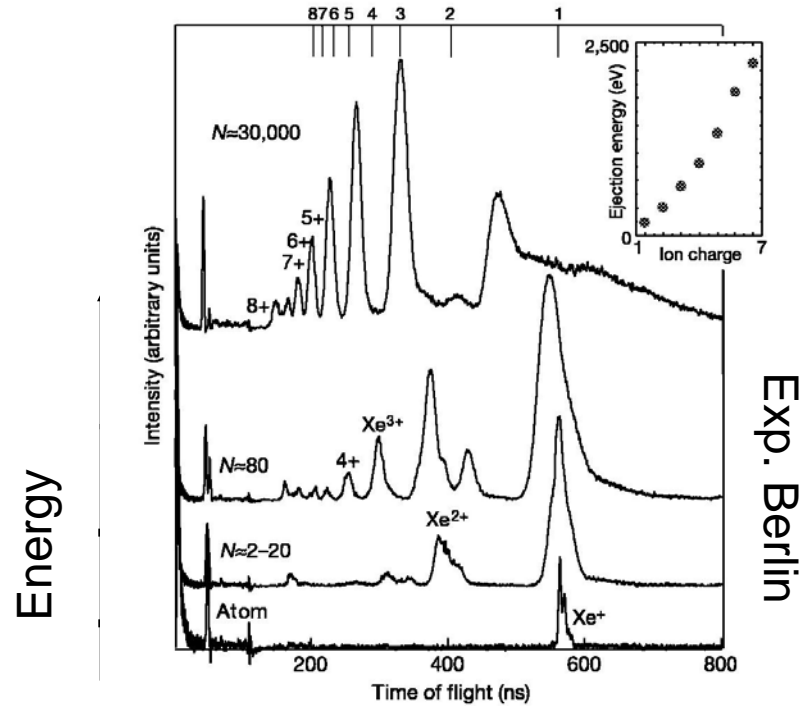


# VUV-FEL dynamics

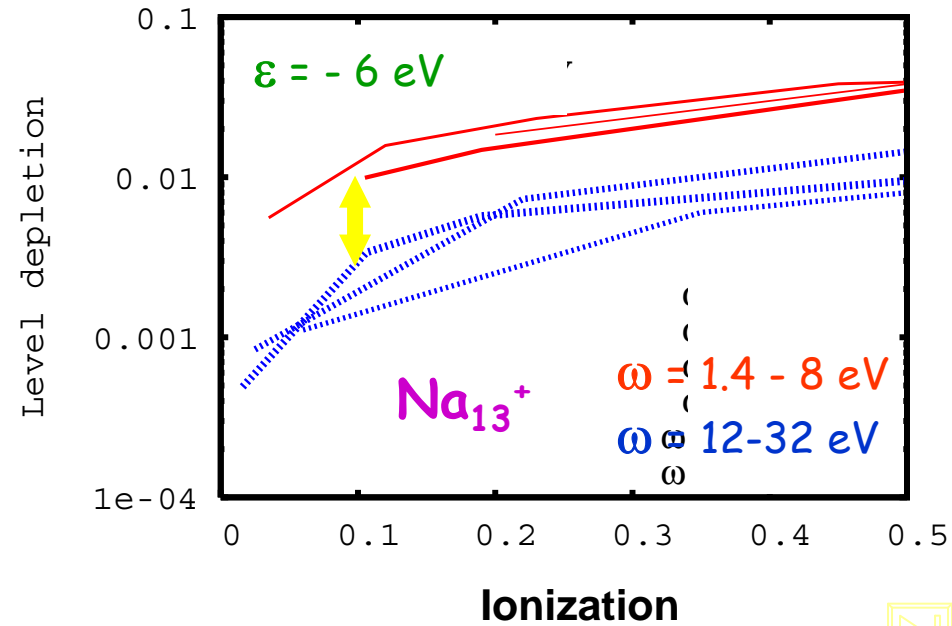
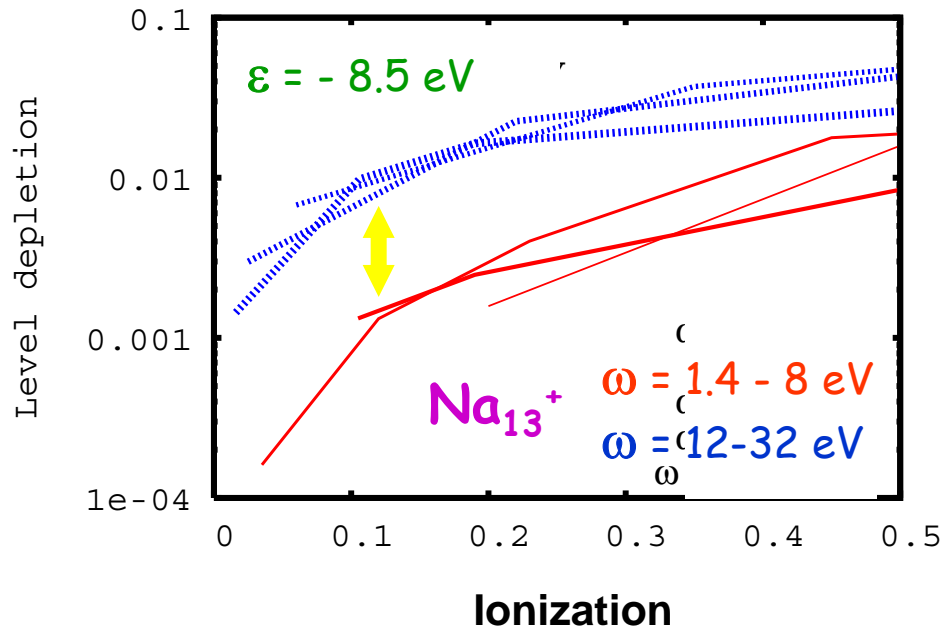
## FEL ionization

How many electrons are emitted from a given level ?

$\omega = 1.4 - 32 \text{ eV}$



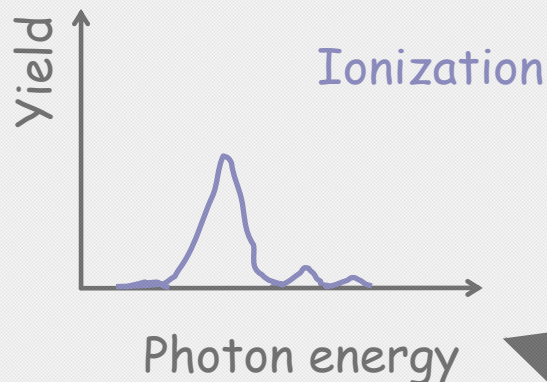
Exp. Berlin



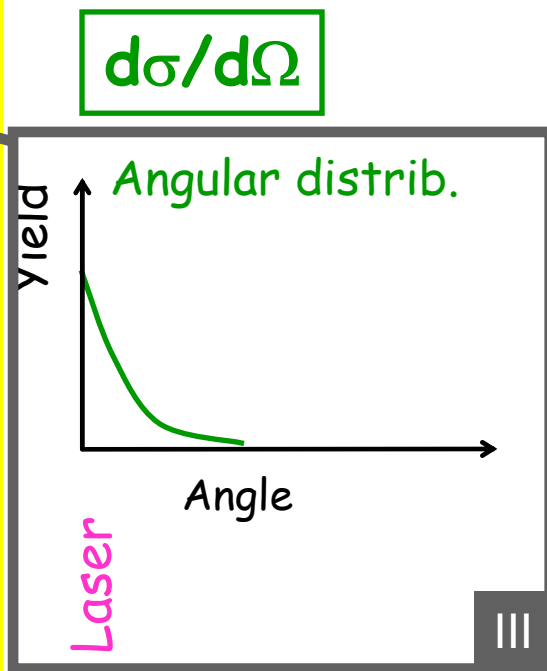
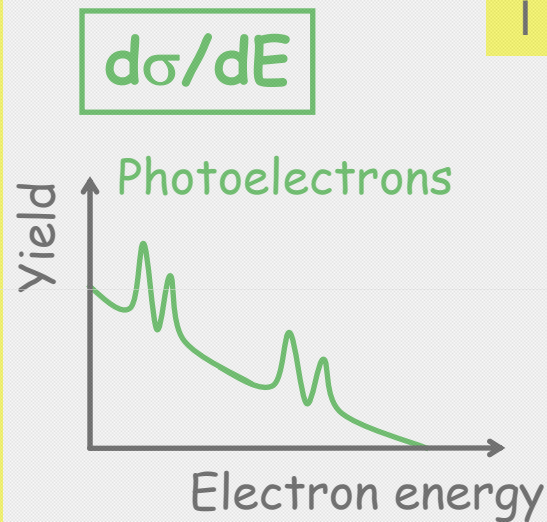
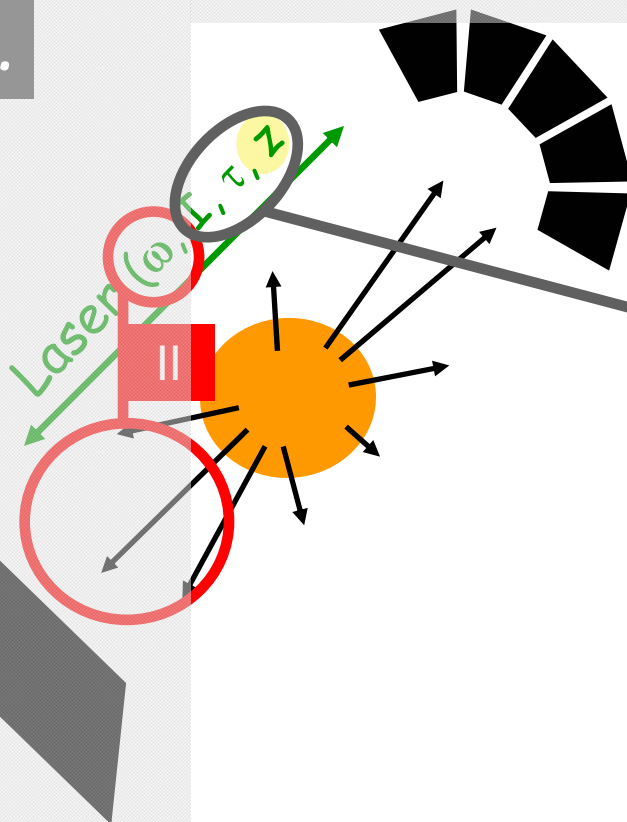
# Electron emission from irradiated clusters

Optical laser - Moderate intensity

Correlations...



$$\sigma(\omega)$$

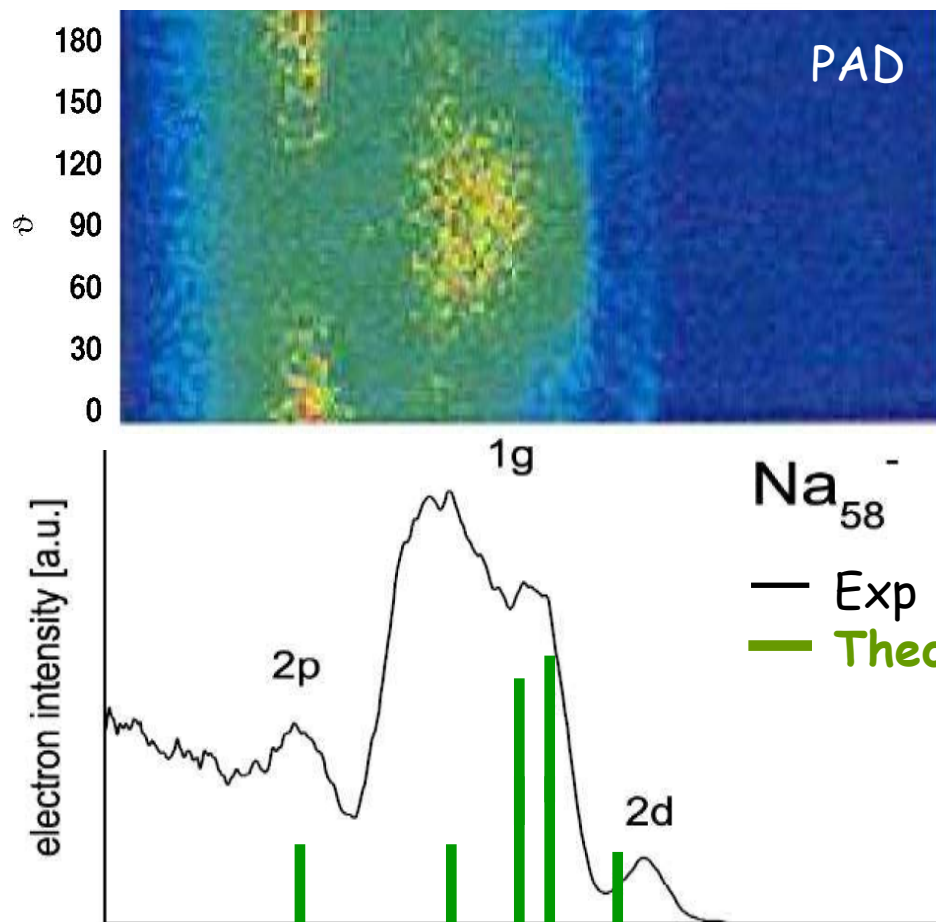
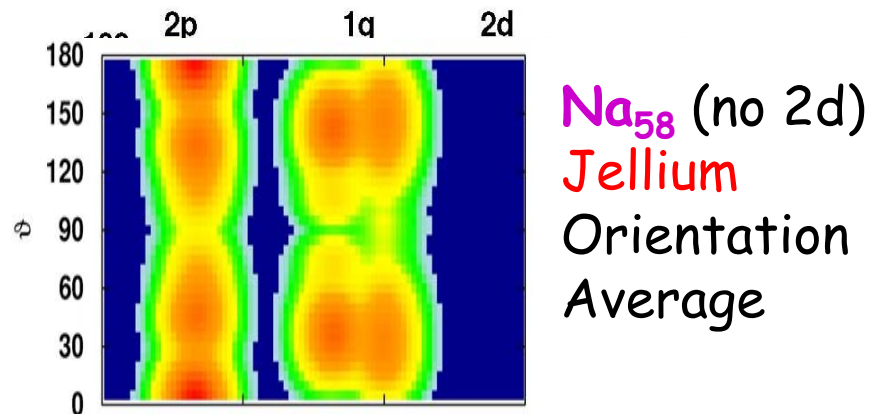
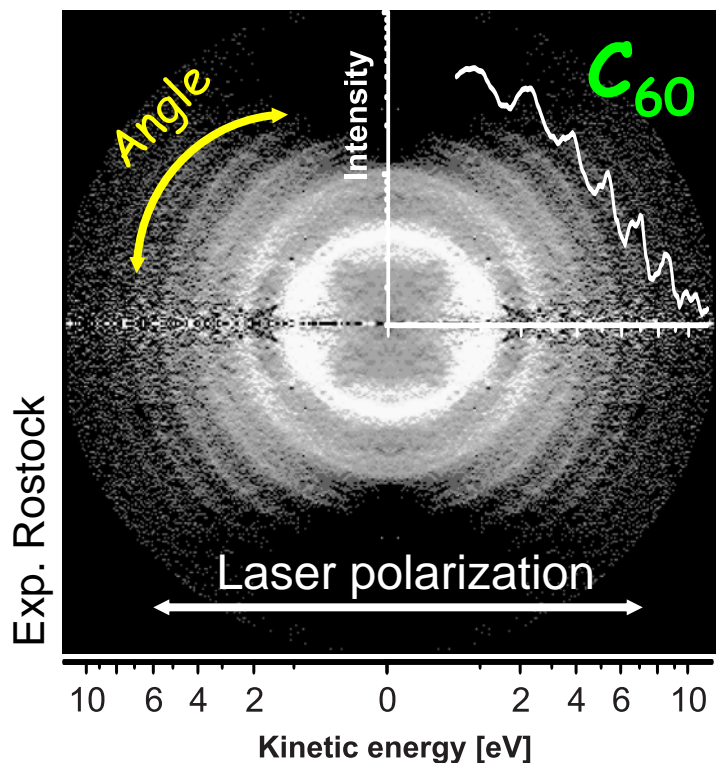


# Energy resolved angular distributions

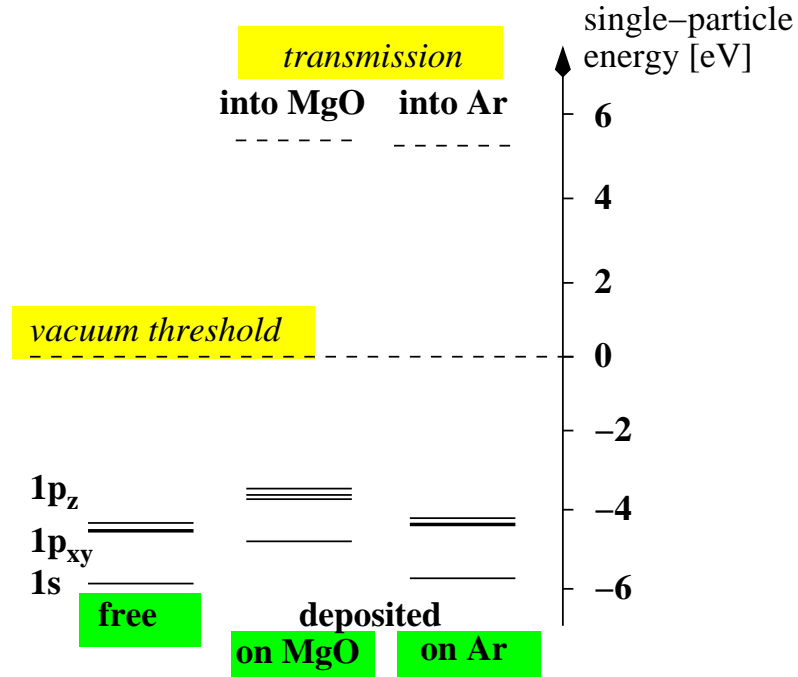
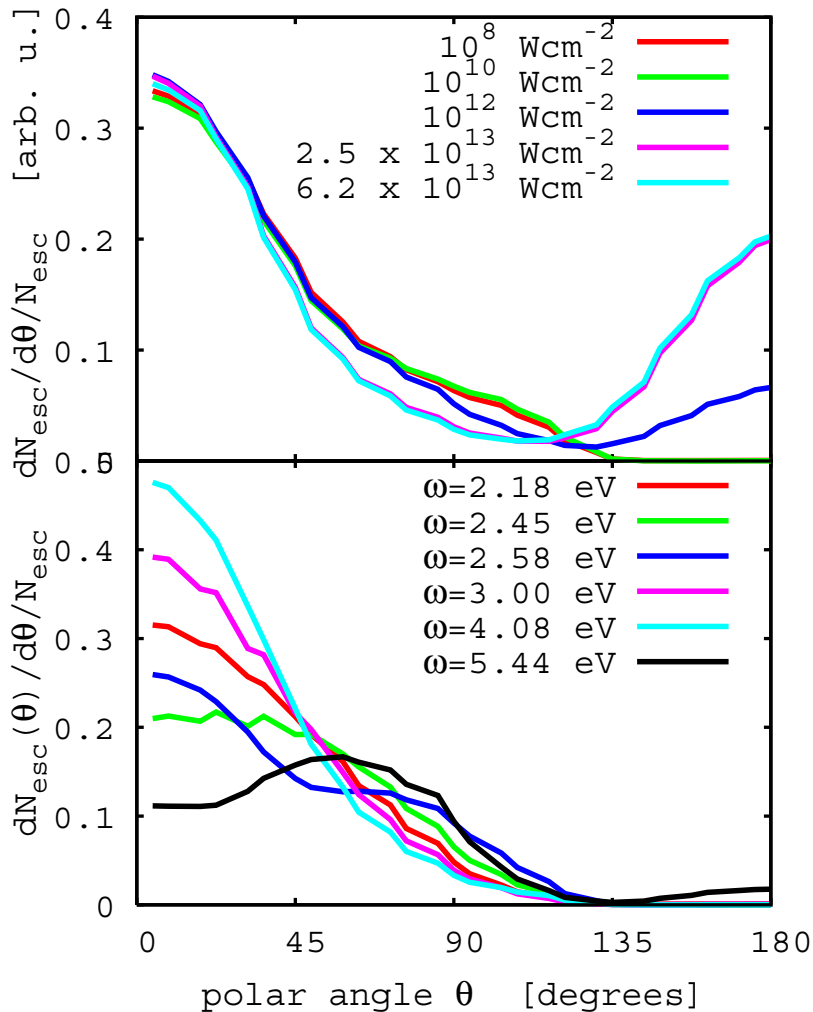
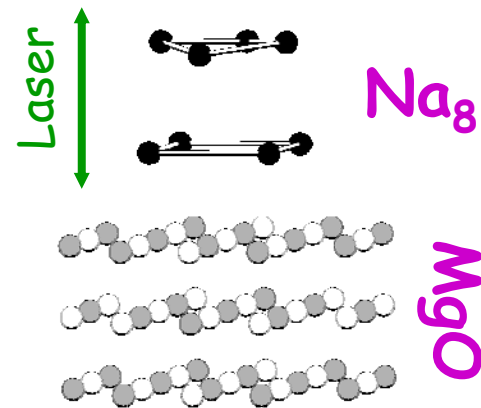
The orientation Problem...

Angle-energy correlation

→  $d\sigma/d\Omega dE$



# Deposited clusters: simpler?



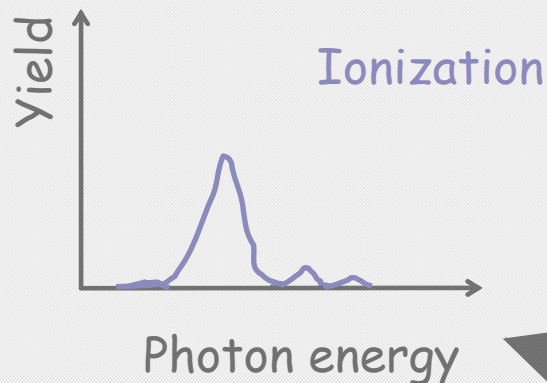
No orientation problem ... but  
 Complex interactions



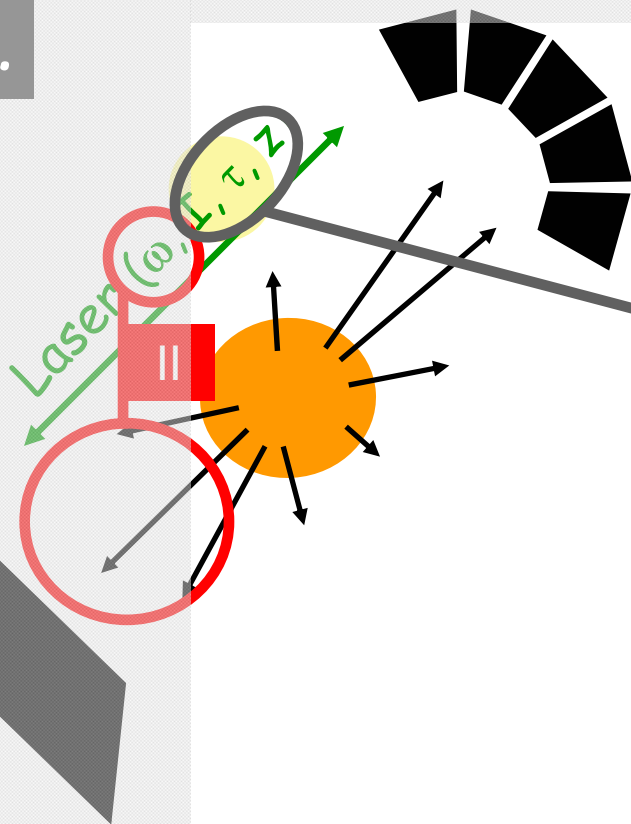
# Electron emission from irradiated clusters

Optical laser - Moderate intensity

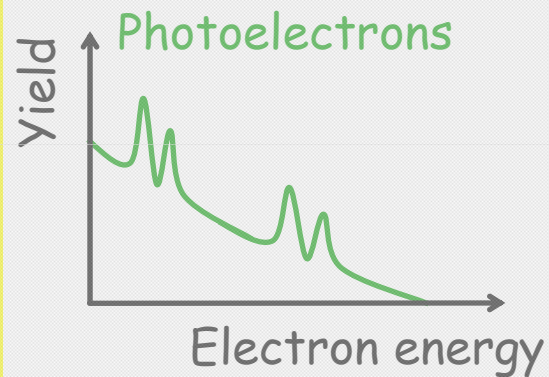
Correlations...



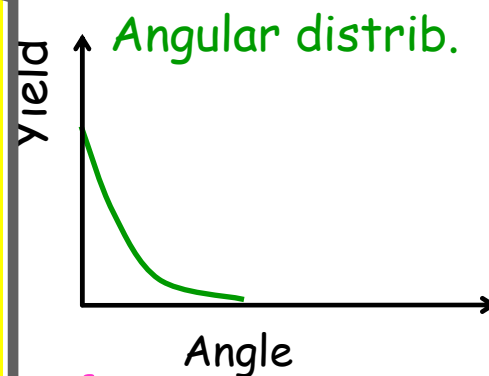
$$\sigma(\omega)$$



$$d\sigma/dE$$



$$d\sigma/d\Omega$$





# Electron-electron dynamics beyond TDLDA

- Complement mean field (TDLDA) by dynamical 2 - body effects




$i\hbar\dot{\rho} = [h, \rho]$	TDLDA	
$\dot{f} = \{h, f\}$	Vlasov	Phase space $f(\mathbf{r}, \mathbf{p}, t)$
$\dot{f} = \{h, f\} + I_{coll}[f]$	VUU	

- Semi classical kinetic equation (plasma, nuclear physics ...)
- Collision integral

$$I_{coll}[f] \sim \int d\mathbf{p}_2 d\mathbf{p}_3 d\mathbf{p}_4 \delta(\sum \mathbf{p}_i) \delta(\sum \epsilon_i) \frac{d\sigma}{d\Omega} \{f_1 f_2 (1 - f_3)(1 - f_4) - \dots\}$$

Screened Coulomb cross section integral

Pauli blocking

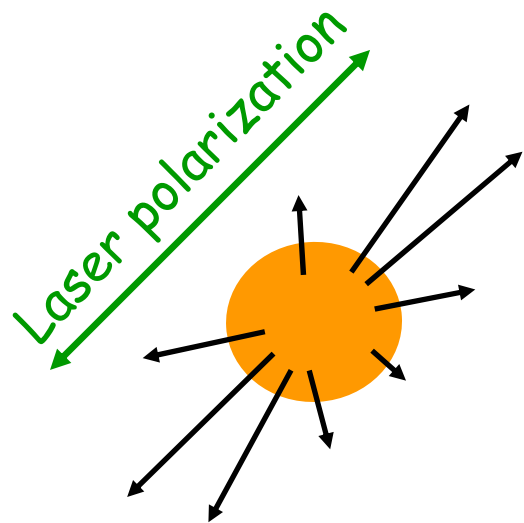


$$V(r) \sim \frac{e^2}{r} \exp(-r/r_0) \quad r_0 \sim 3a_0$$

Numerics from test particles



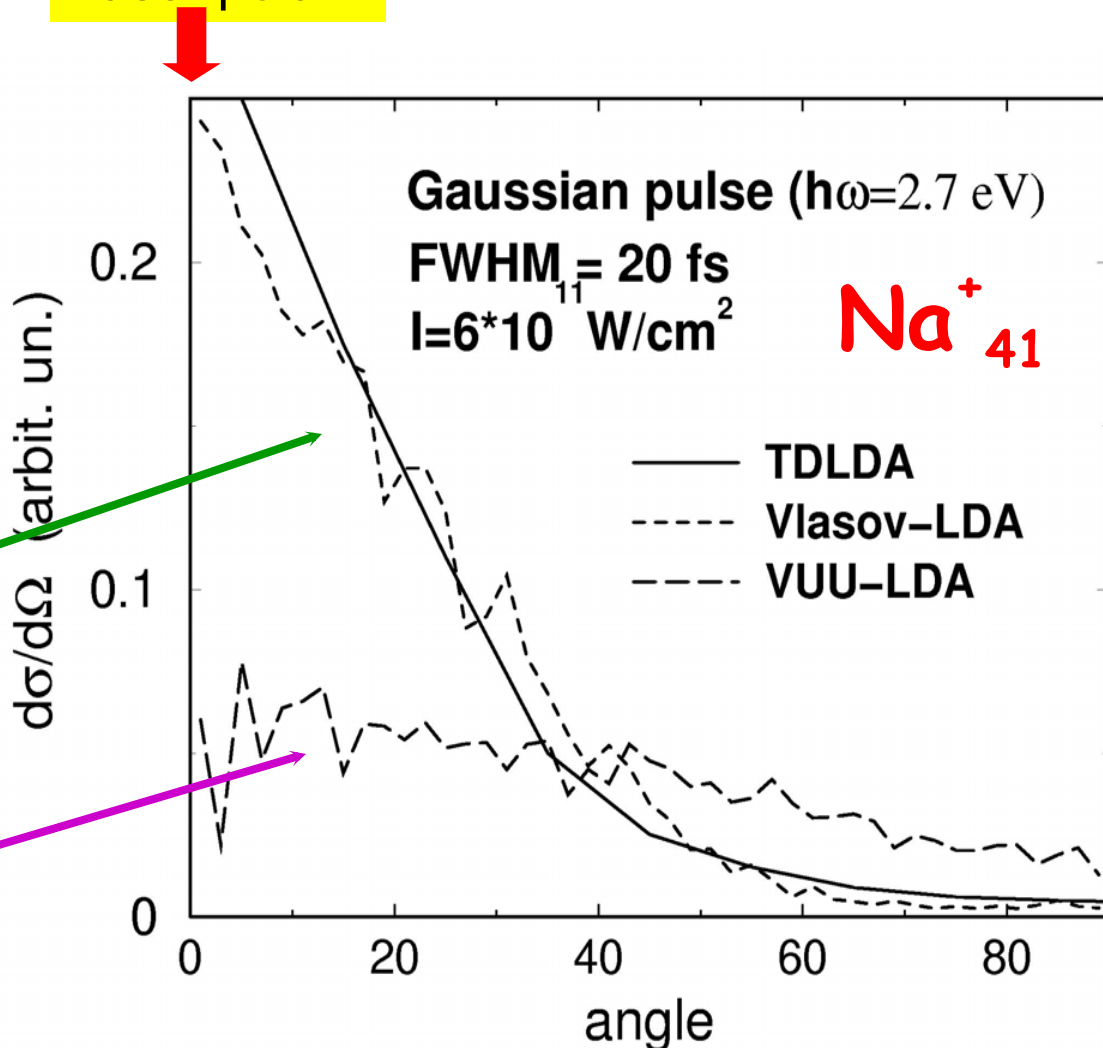
# Angular distributions of photoelectrons



Laser polar.

Mean field:  
Directed emission

Mean-field + colls :  
Isotropic emission





# Some conclusions and perspectives

## ➤ The various facets of electron emission

Photoelectron spectroscopy

Angular distributions of photoelectrons

FEL ionization dynamics

## ➤ Many other research directions

- Formal aspects

Ex: quantum vs classical, extended mean field, SIC ...

- Clusters in laser fields

Ex: pump/probe dynamics, high intensity lasers ...

- Dynamics of deposited and embedded clusters

Ex: Na@Ar, towards defect formation in solids ...

- Towards systems of biological interest

Ex: irradiation (laser, ion) of organic molecules ...

