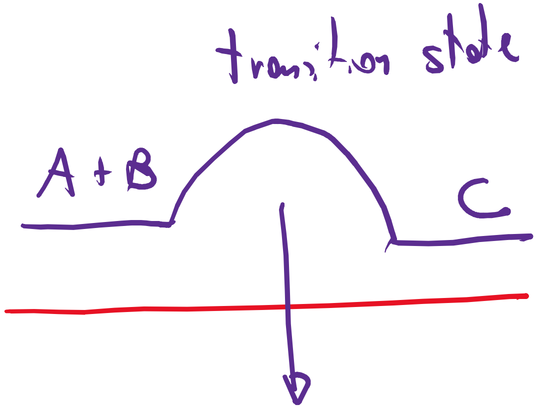
# Misure di dinamiche elettroniche

## Introduzione a spettroscopie Pump & Probe

- Le fotoemissione risonante → 0 - 80 fs (dinamiche ultra-veloci)




tempo caratteristico di durata del transition state: $\approx$ 1 ps

Ossidazione di CO su Ru

Abbiamo visto $O_2$, $CO$ su Pd

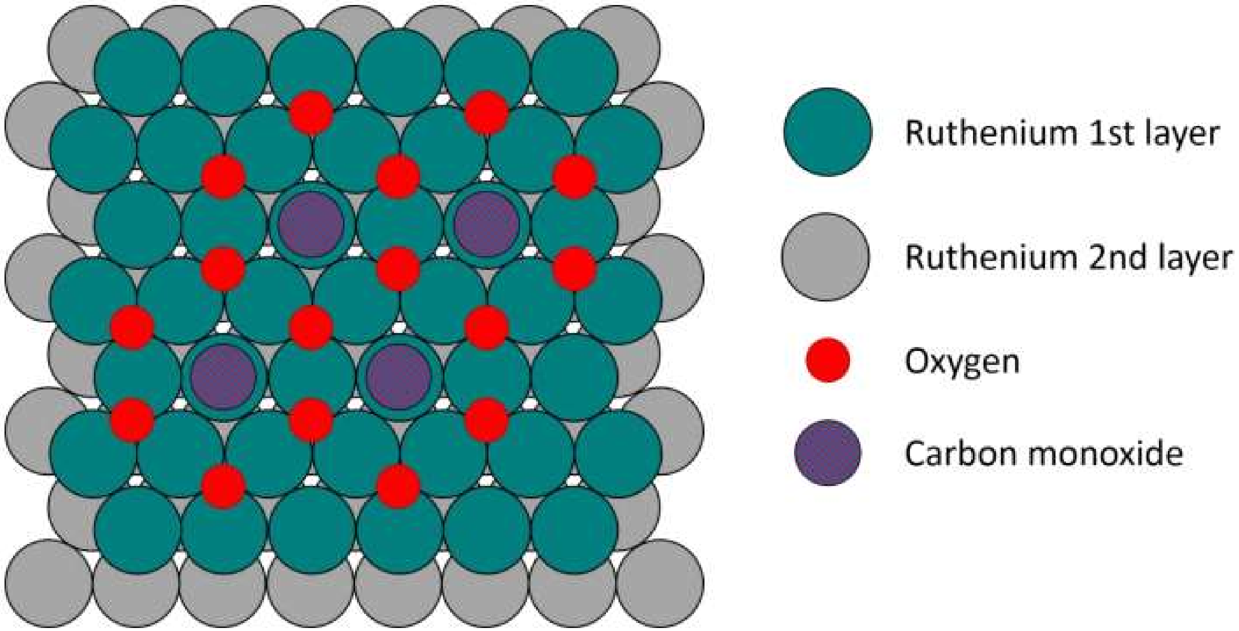
Ru (100)

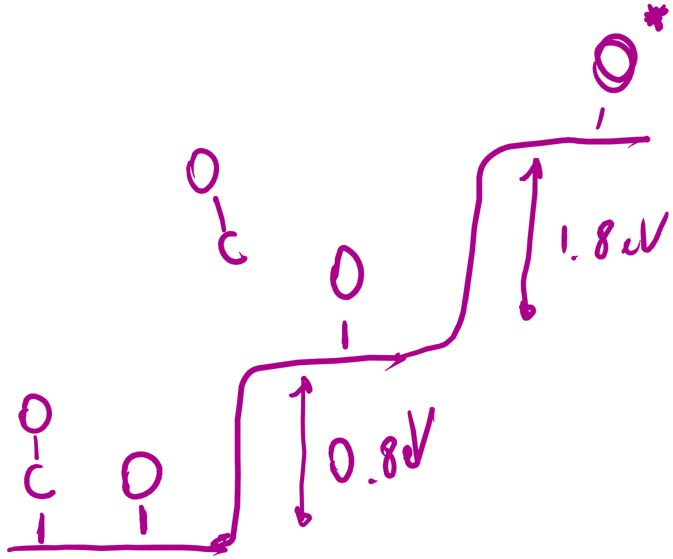
$CO + \frac{1}{2} O_2 \Rightarrow CO_2$

$A + B \Rightarrow C$

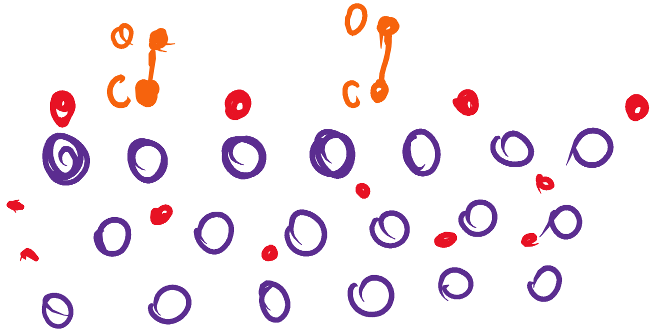
1. $O_2 \rightarrow 2O$
2. $CO$
3. scaldo il campione
4. → ottengo $CO_2$

ok, Pt, Pd



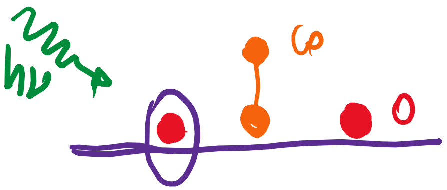



- Se su Ru deposito "molto" $O_2$ ;




→ cambia la chimica di adsorbimento di O in superficie → l'O di superficie diventa più facilmente attivabile.

# Fotocatalisi

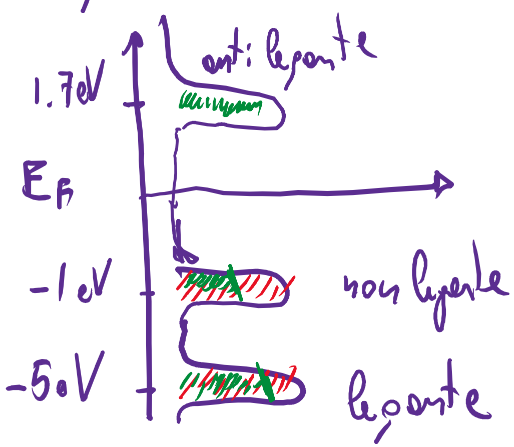


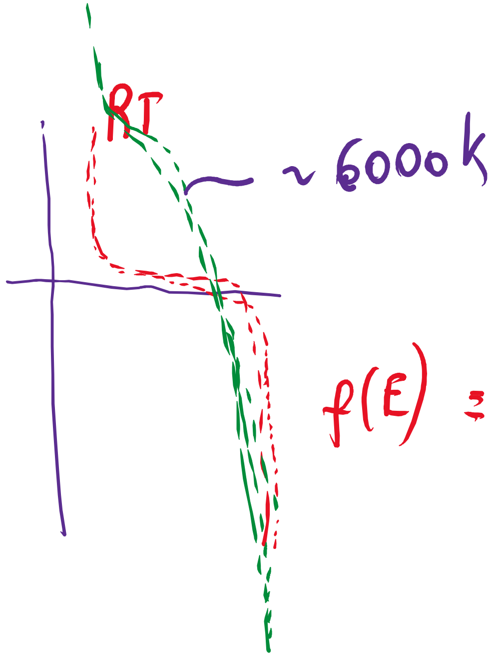

- mando pacchetto di fotoni hν
- → genero una nuvola di $e^-$
- → modifico la distribuzione data da $f(E)$

**Hot electrons** vivono ~ 1 ps

⇒ indebolisco il legame Ru - O

⇒ $O^*$ $e^-$ + facile da ottenere (in questo caso ho proprio $O^*$)




$$f(E) = \frac{1}{e^{\frac{E-E_F}{kT}}+1}$$

Lo stato antilegante viene parzialmente riempito con un impulso di fotoni e la relativa Te=6000K. Lo stesso impulso provoca un parziale svuotamento del primo orbitale occupato, che però ha carattere non legante.

Complessivamente, l'impulso di fotoni indebolisce il legame O-Ru e mette l'ossigeno in uno stato attivo per l'ossidazione di CO che gli sta accanto

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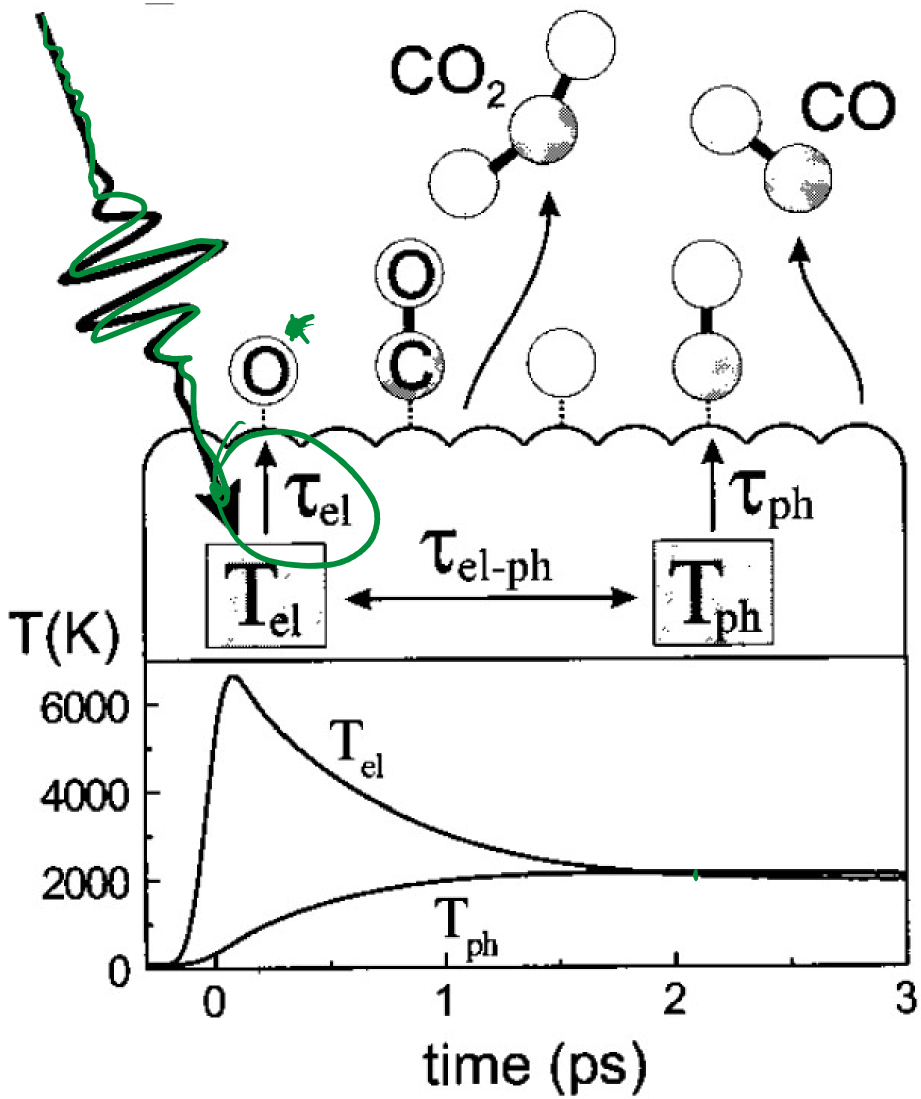
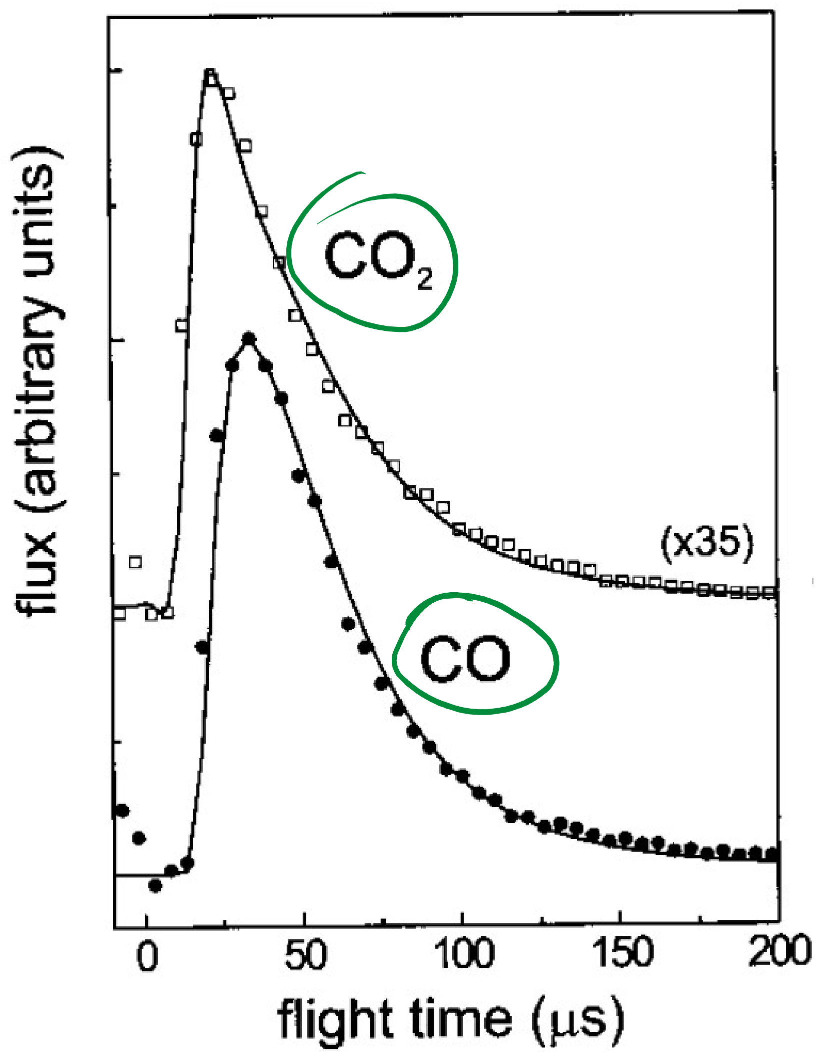
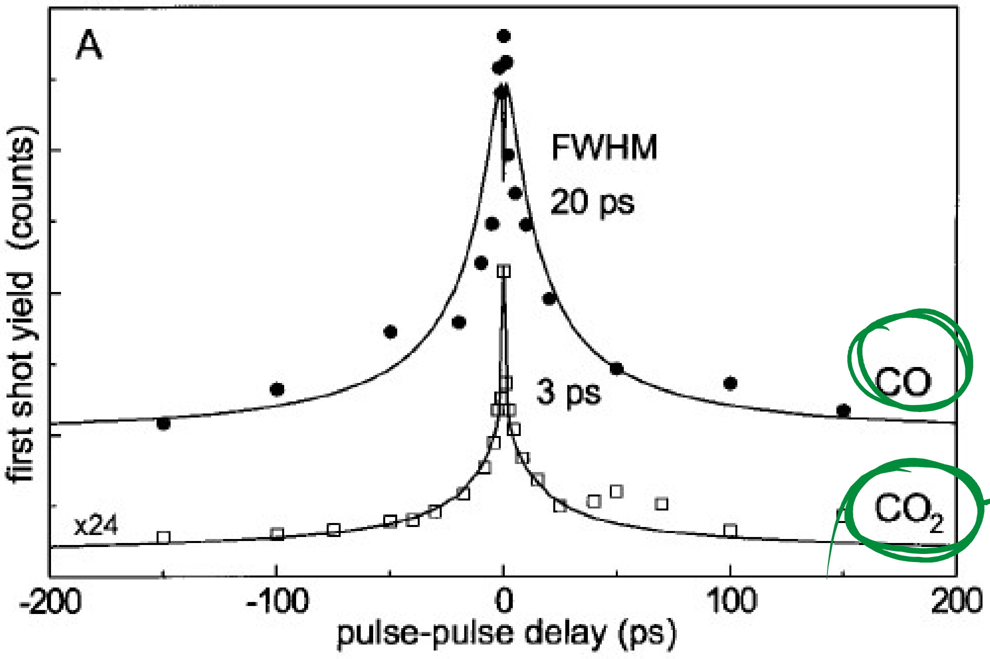
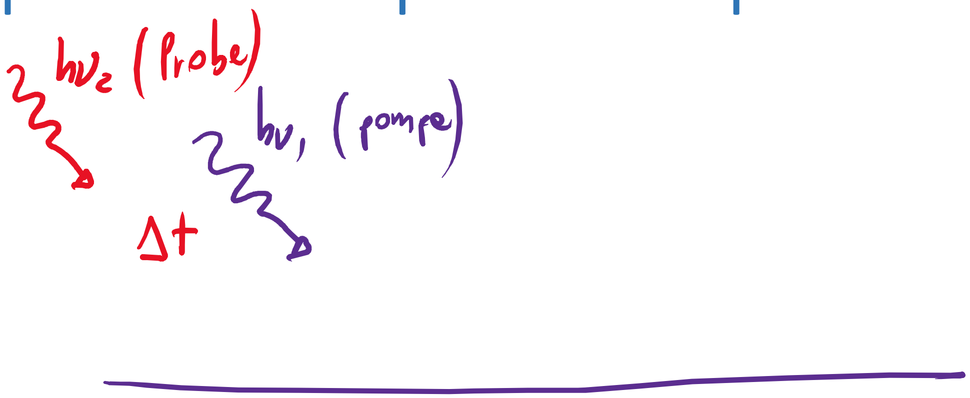

CO2
CO
O
O
C
τel
τph
τel-ph
Tel
Tph
T(K)
6000
4000
2000
0
Tel
Tph
0
1
2
3
time (ps)


flux (arbitrary units)
CO2
(x35)
CO
0
50
100
150
200
flight time (μs)




è un processo veloce, legato agli hot electrons

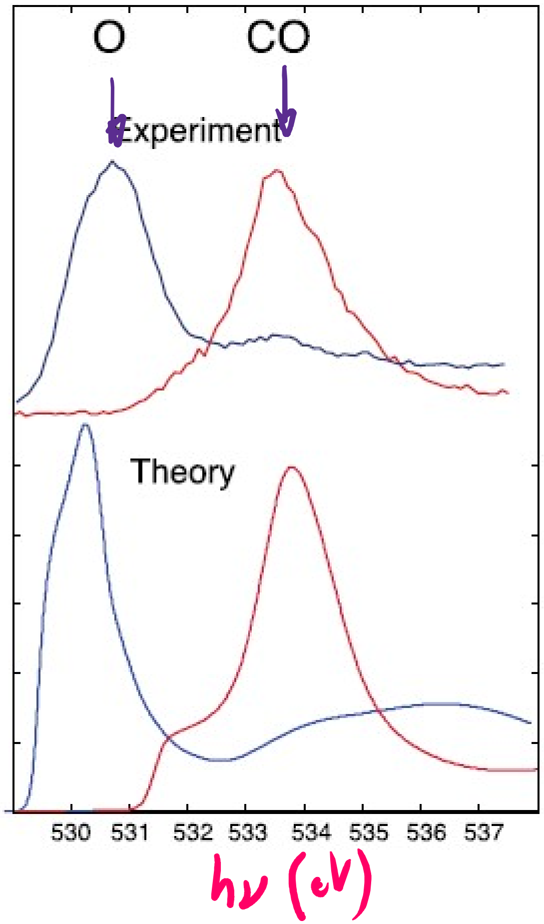
# Spettroscopia Pump&Probe

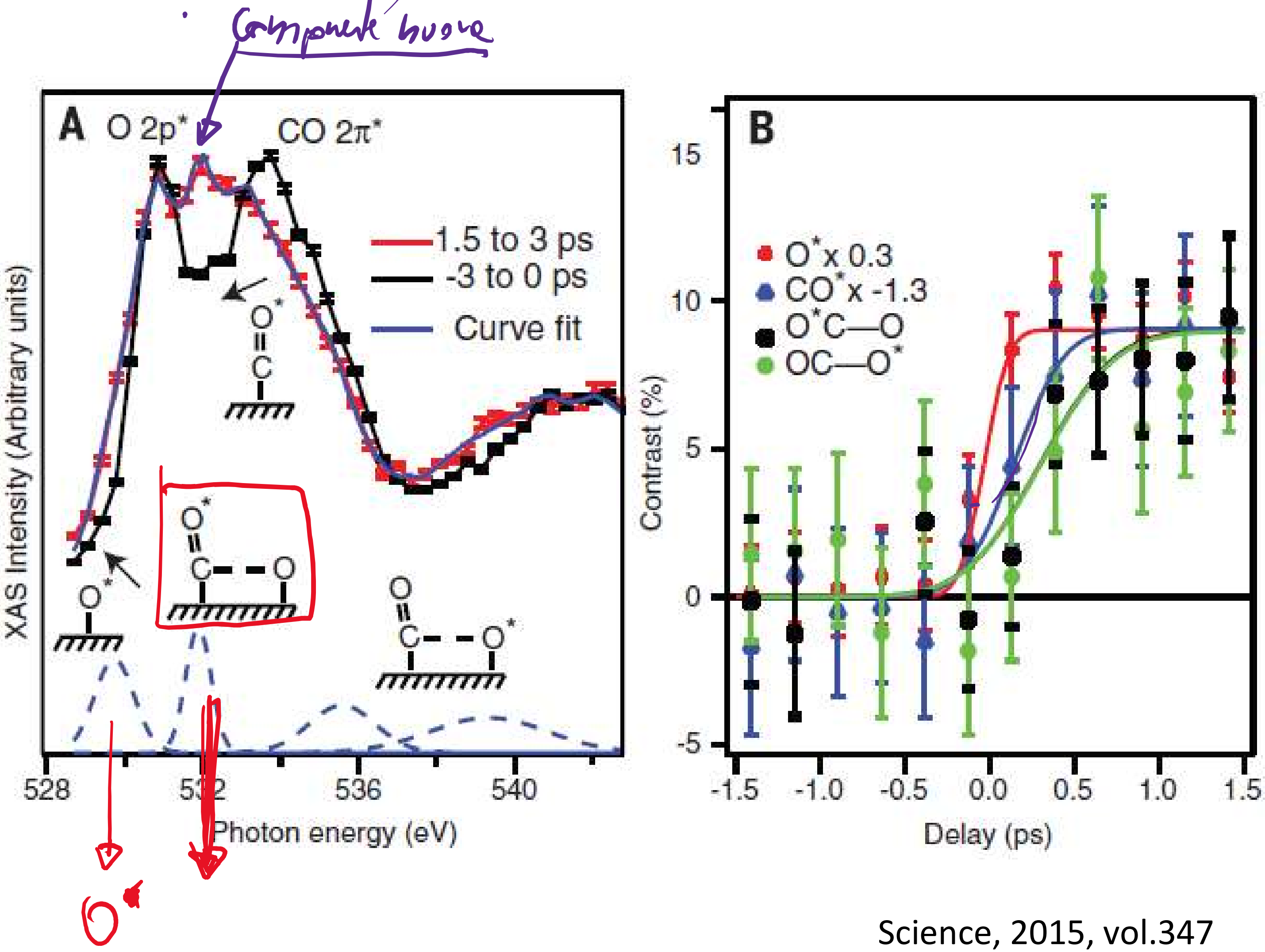



1. porto il sistema in stato eccitato
2. Misure (XPS, NEXAFS...)

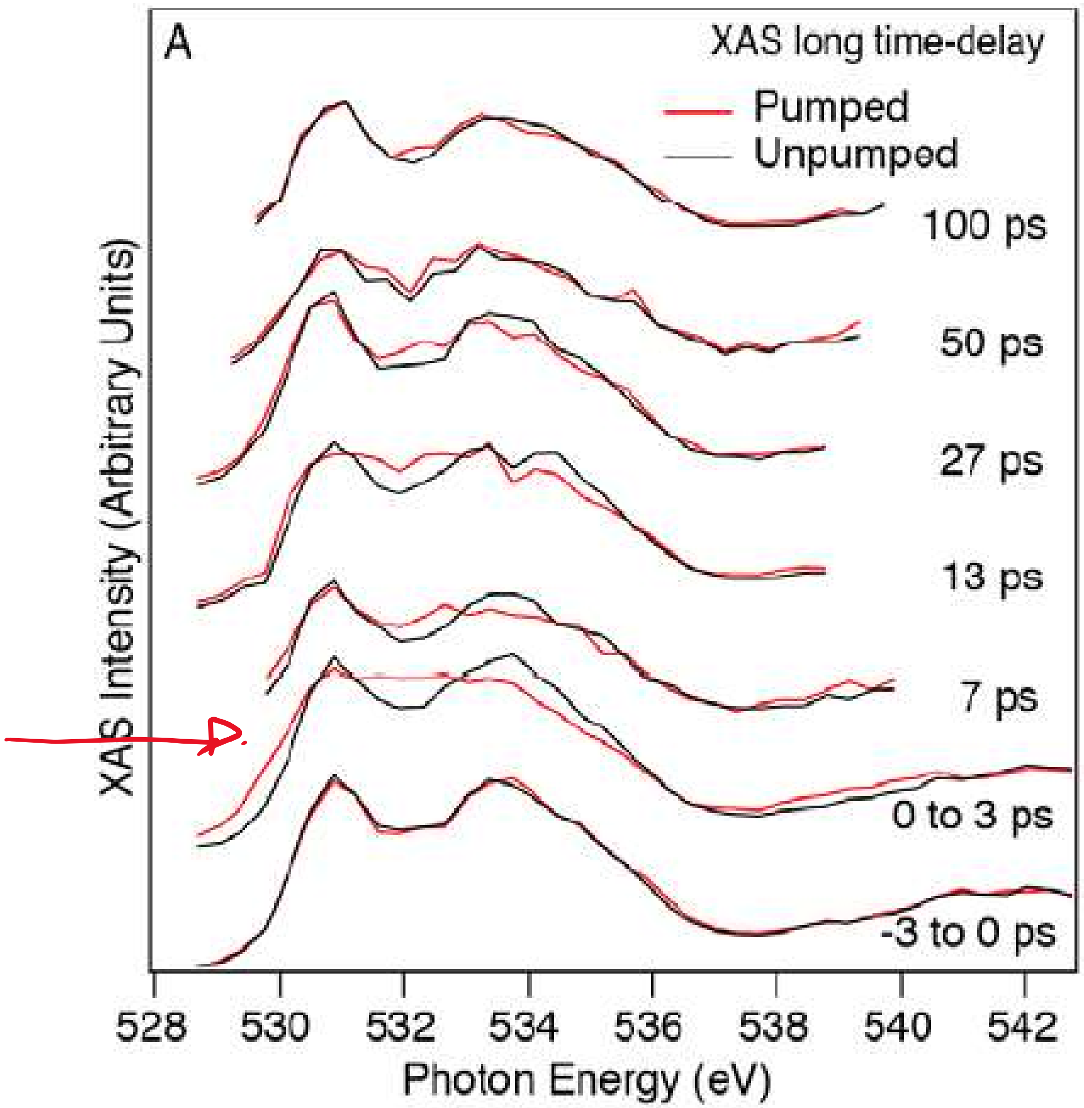
hν1 → crea hot electrons (400 nm)

hν2 → NEXAFS O1s (~530 eV attraversando la soglia)

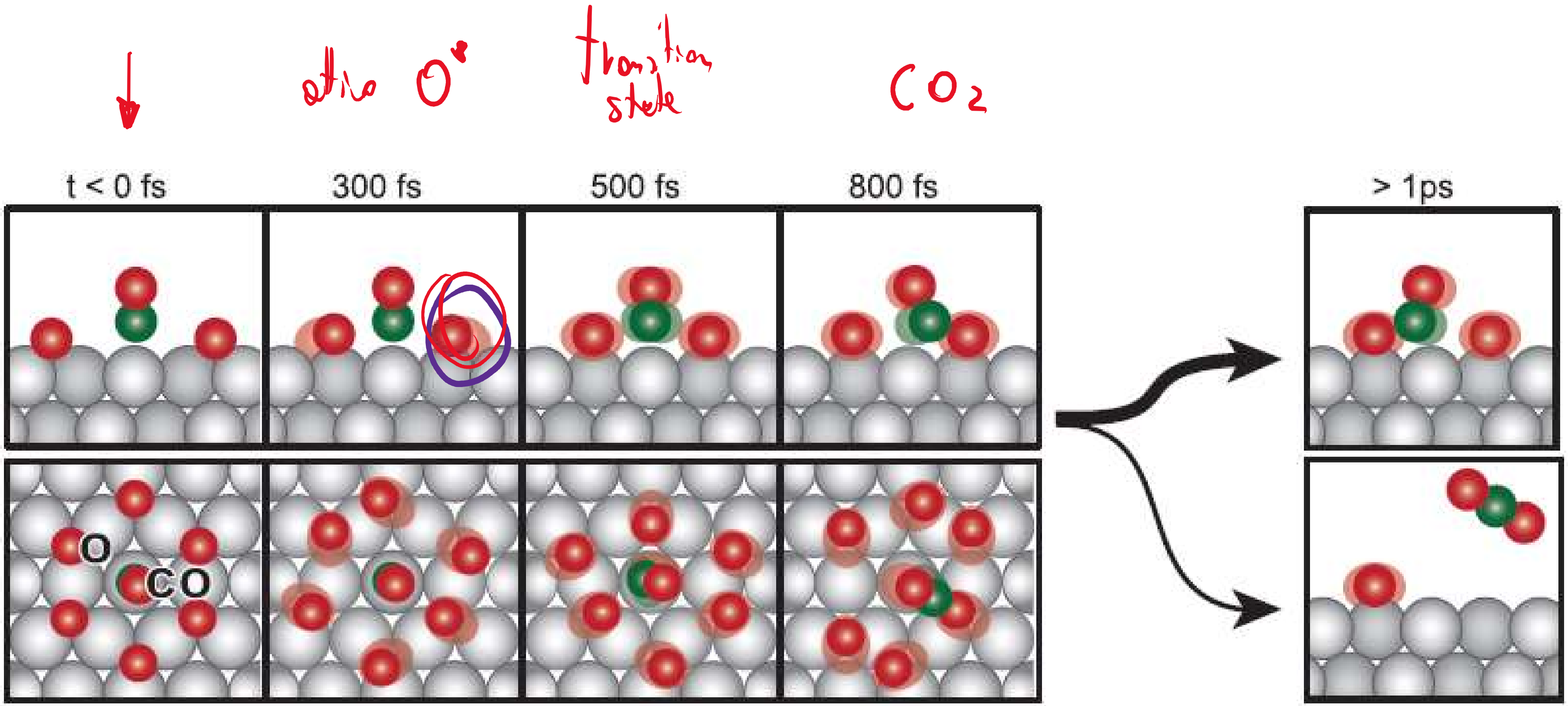



Science, 2015, vol.347




Science, 2015, vol.347

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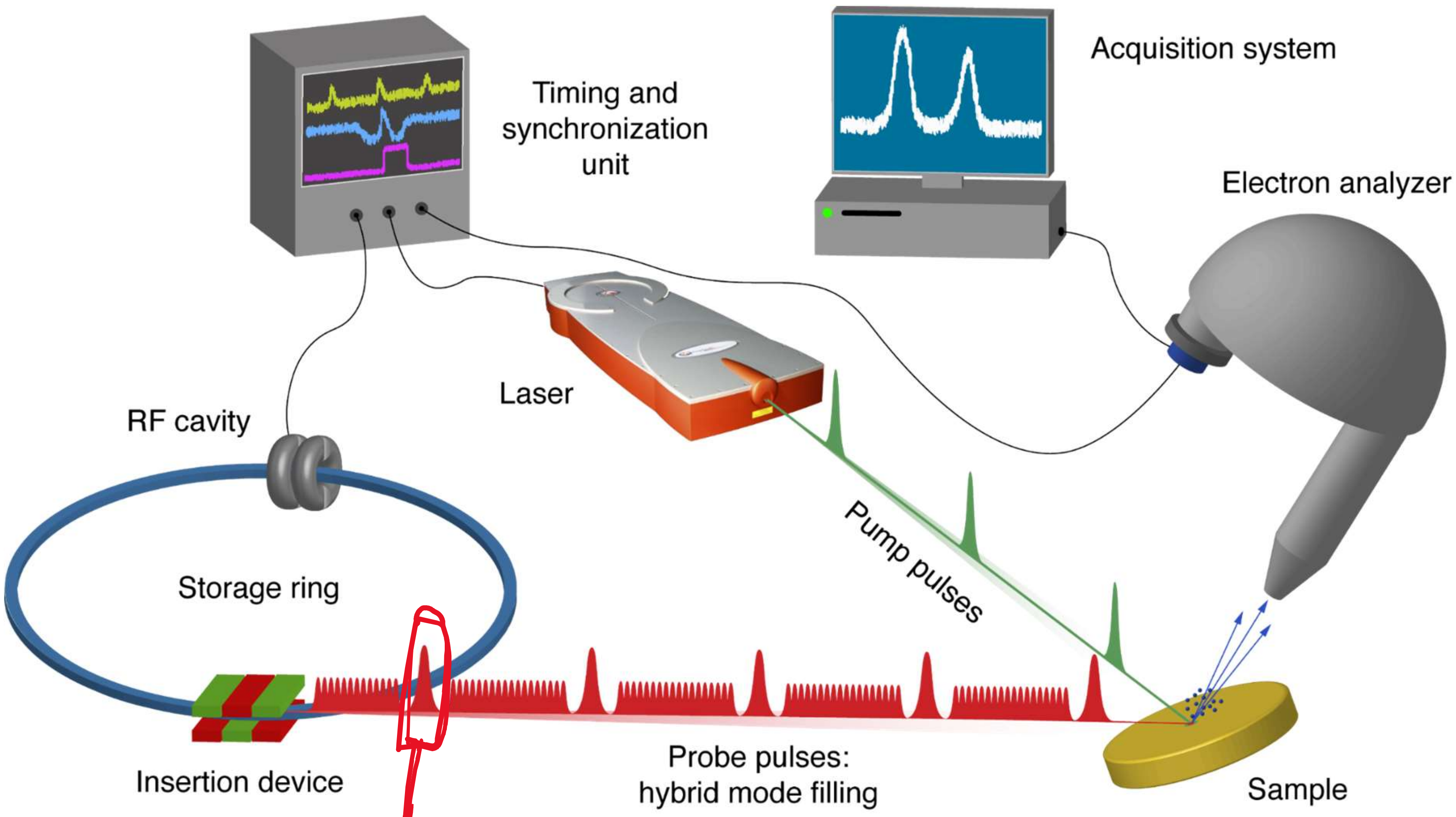
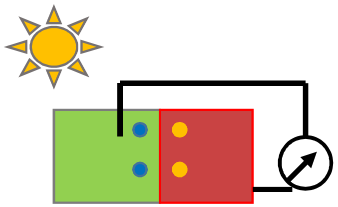
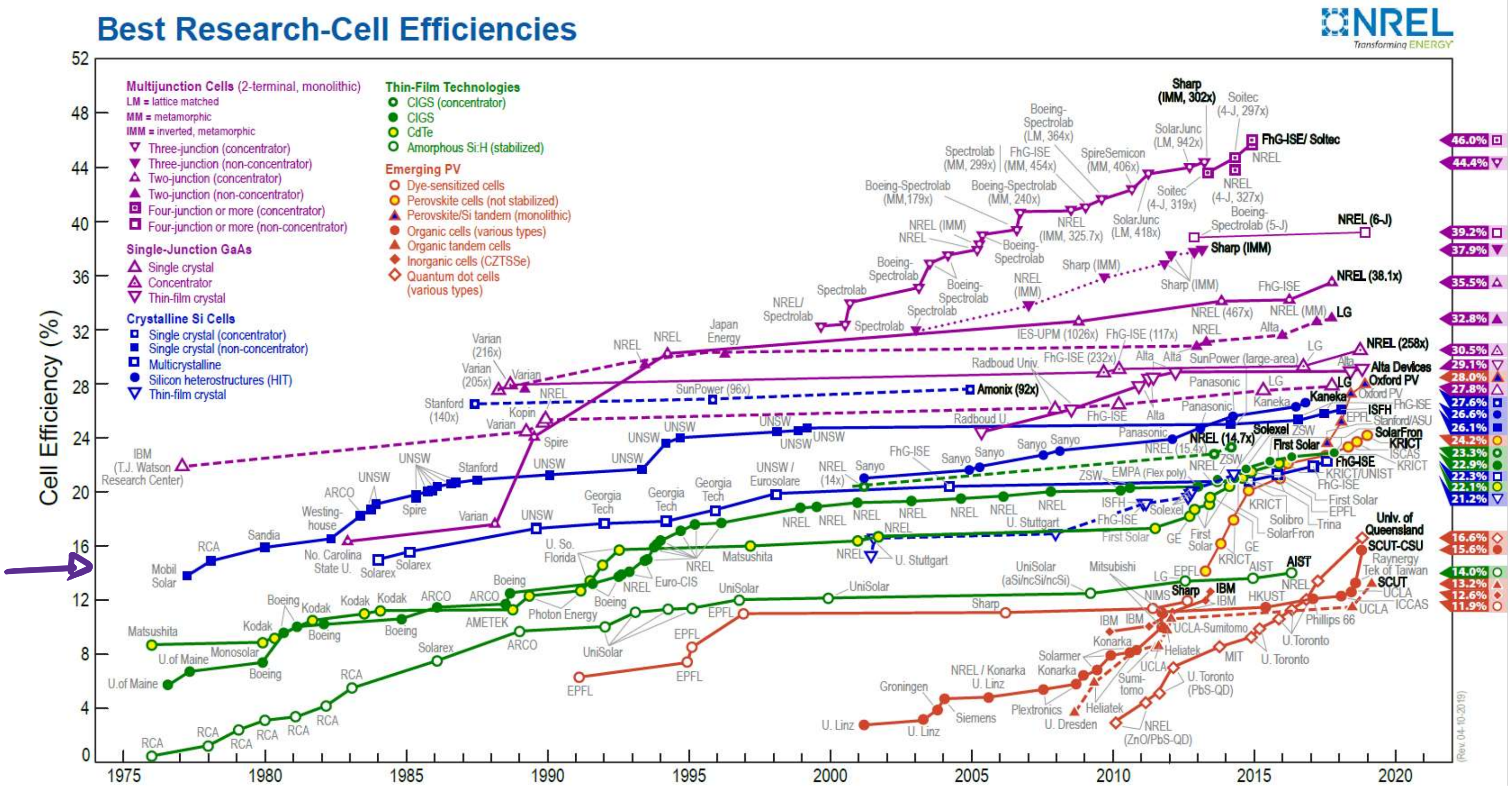
# Experimental Set-Up for Optical Pump-X-ray Probe



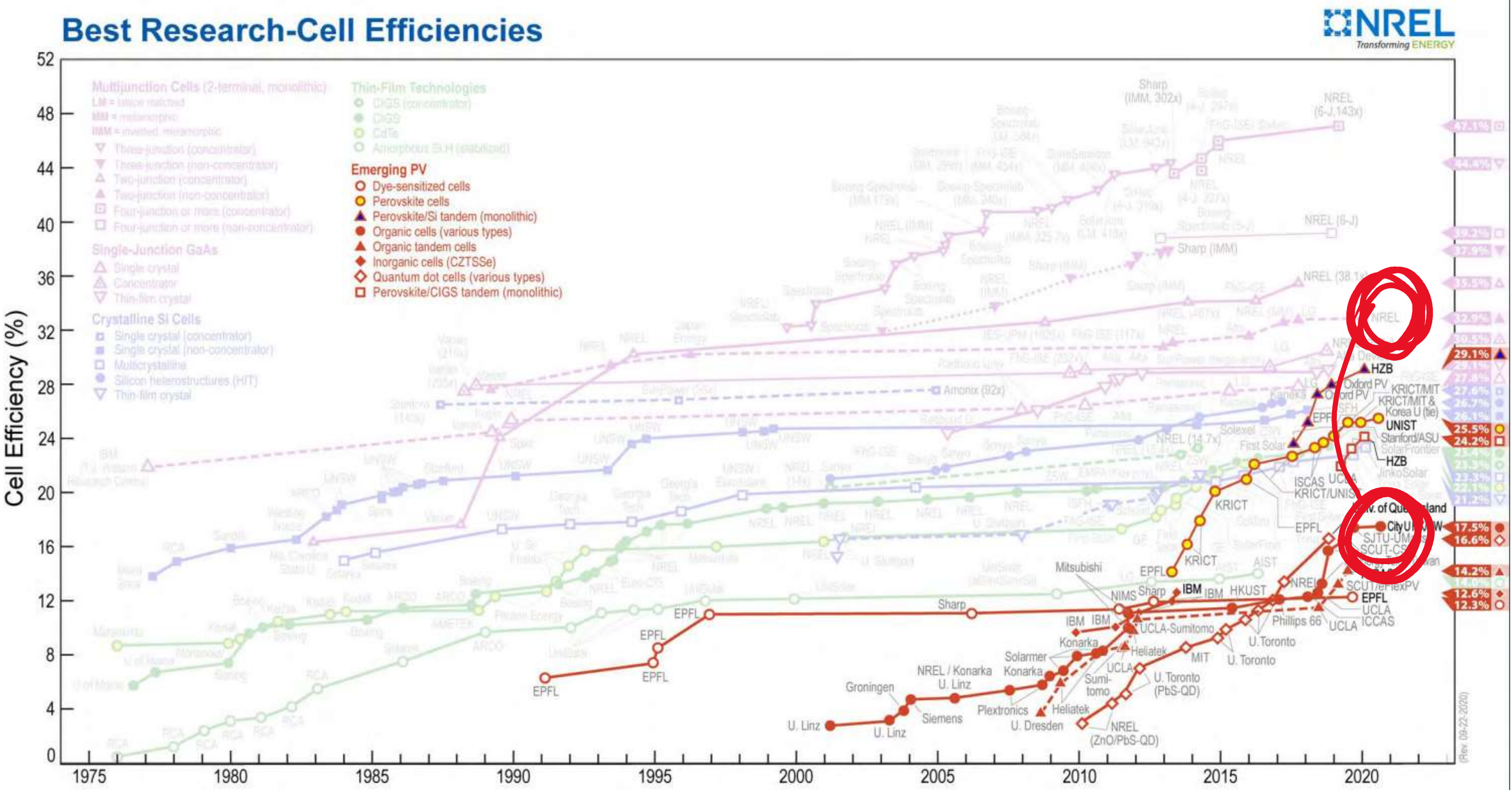

Δt probe sincrotrone ≈ 100 ps → Elettra 2.0 1 ps

# Solar Cells



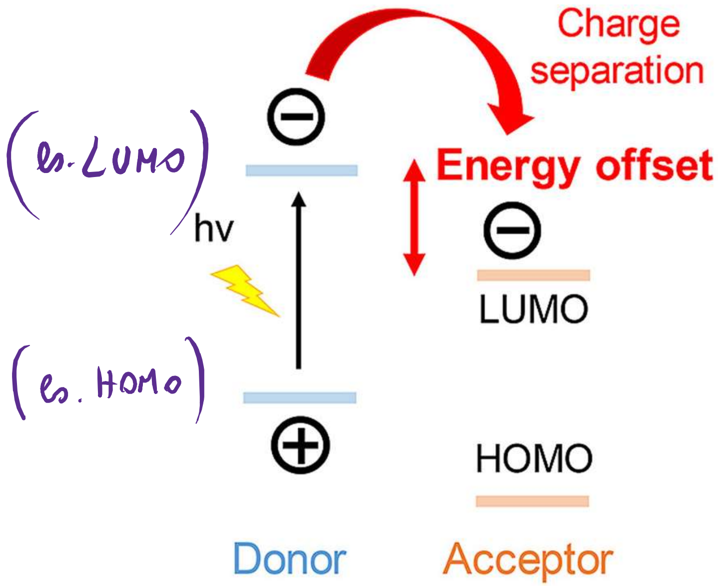


Best Research-Cell Efficiencies
NREL
Transforming ENERGY
Cell Efficiency (%)
Multijunction Cells (2-terminal, monolithic)
LM = lattice matched
MM = metamorphic
IMM = inverted, metamorphic
Three-junction (concentrator)
Three-junction (non-concentrator)
Two-junction (concentrator)
Two-junction (non-concentrator)
Four-junction or more (concentrator)
Four-junction or more (non-concentrator)
Single-Junction GaAs
Single crystal
Concentrator
Thin-film crystal
Crystalline Si Cells
Single crystal (concentrator)
Single crystal (non-concentrator)
Multicrystalline
Silicon heterostructures (HIT)
Thin-film crystal
Thin-Film Technologies
CIGS (concentrator)
CIGS
CdTe
Amorphous Si:H (stabilized)
Emerging PV
Dye-sensitized cells
Perovskite cells (not stabilized)
Perovskite/Si tandem (monolithic)
Organic cells (various types)
Organic tandem cells
Inorganic cells (CZTSSe)
Quantum dot cells (various types)
46.0%
44.4%
39.2%
37.9%
35.5%
32.8%
30.5%
29.1%
28.0%
27.8%
27.6%
26.6%
26.1%
24.2%
23.3%
22.9%
22.3%
22.1%
21.2%
16.6%
15.6%
14.0%
13.2%
12.6%
11.9%
1975
1980
1985
1990
1995
2000
2005
2010
2015
2020

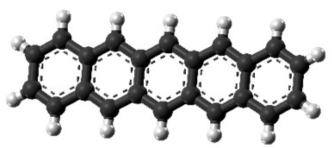


Best Research-Cell Efficiencies
NREL
Transforming ENERGY
Cell Efficiency (%)
52
48
44
40
36
32
28
24
20
16
12
8
4
0
1975
1980
1985
1990
1995
2000
2005
2010
2015
2020
Multijunction Cells (2-terminal, monolithic)
Thin-Film Technologies
Single-Junction GaAs
Crystalline Si Cells
Emerging PV
Dye-sensitized cells
Perovskite cells
Perovskite/Si tandem (monolithic)
Organic cells (various types)
Organic tandem cells
Inorganic cells (CZTSSe)
Quantum dot cells (various types)
Perovskite/CIGS tandem (monolithic)
47.1%
44.4%
39.2%
37.9%
35.5%
29.1%
25.5%
24.2%
17.5%
16.6%
14.2%
12.6%
12.3%
HZB
Oxford PV
KRICT/MIT
KRICT/MIT &
Korea U (tie)
UNIST
Stanford/ASU
KRICT
EPFL
IBM
Sharp
Mitsubishi
U. Linz
Siemens
Groningen
NREL / Konarka
U. Linz
Konarka
Solarmer
Plextronics
U. Dresden
Heliatek
NREL
(ZnO/PbS-QD)
U. Toronto
(PbS-QD)
U. Toronto
MIT
UCLA
Phillips 66
ICCAS
SCUT/eFlexPV
HKUST
AIST
(Rev. 09-22-2020)

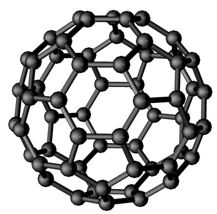
## Giunzione p-n organica




*Organic Electronics 71 (2019) 45–49*



pentacene

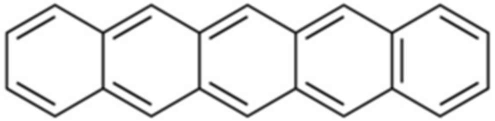


C60

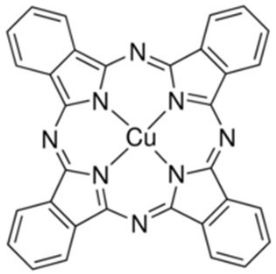
## Bulk heterojunction cells

1. hν viene assorbito dal materiale 1
2. formazione di coppie $e^-$ - lacune **ECCITONE**
3. separazione dell'ECCITONE all'interfaccia
4. trasporto di cariche agli elettrodi (I fotovoltaica)

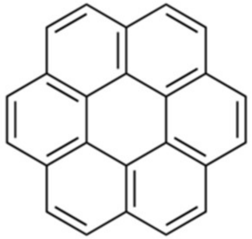
## p-type



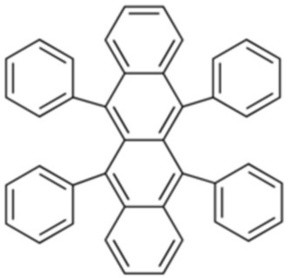
pentacene




CuPc

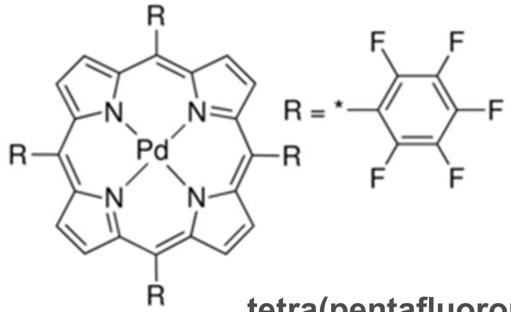


coronene

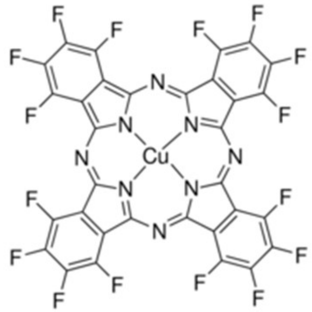


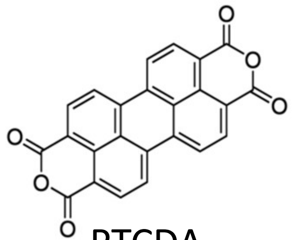
rubrene

## n-type



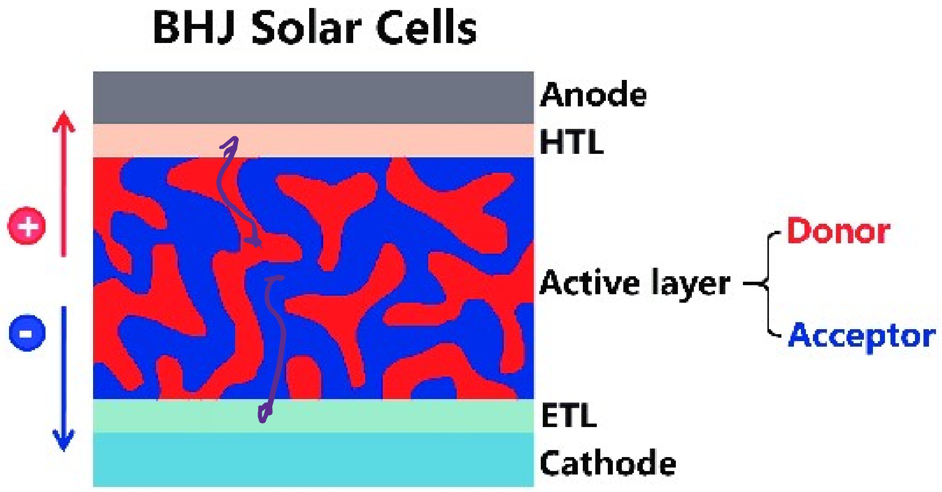

tetra(pentafluorophenyl)porphine

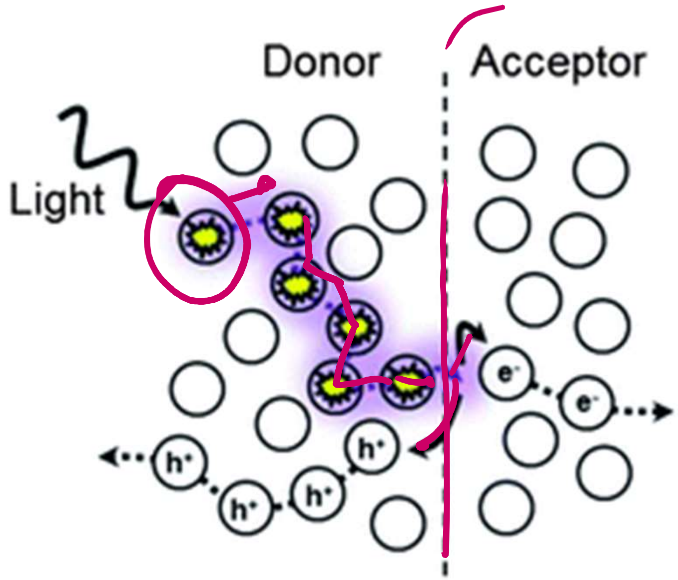


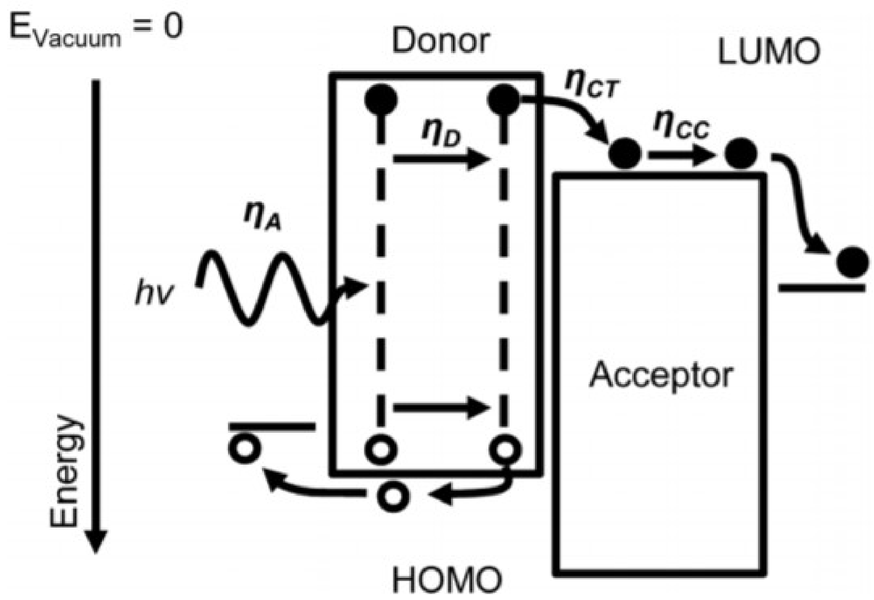




PTCDA


Fullerene

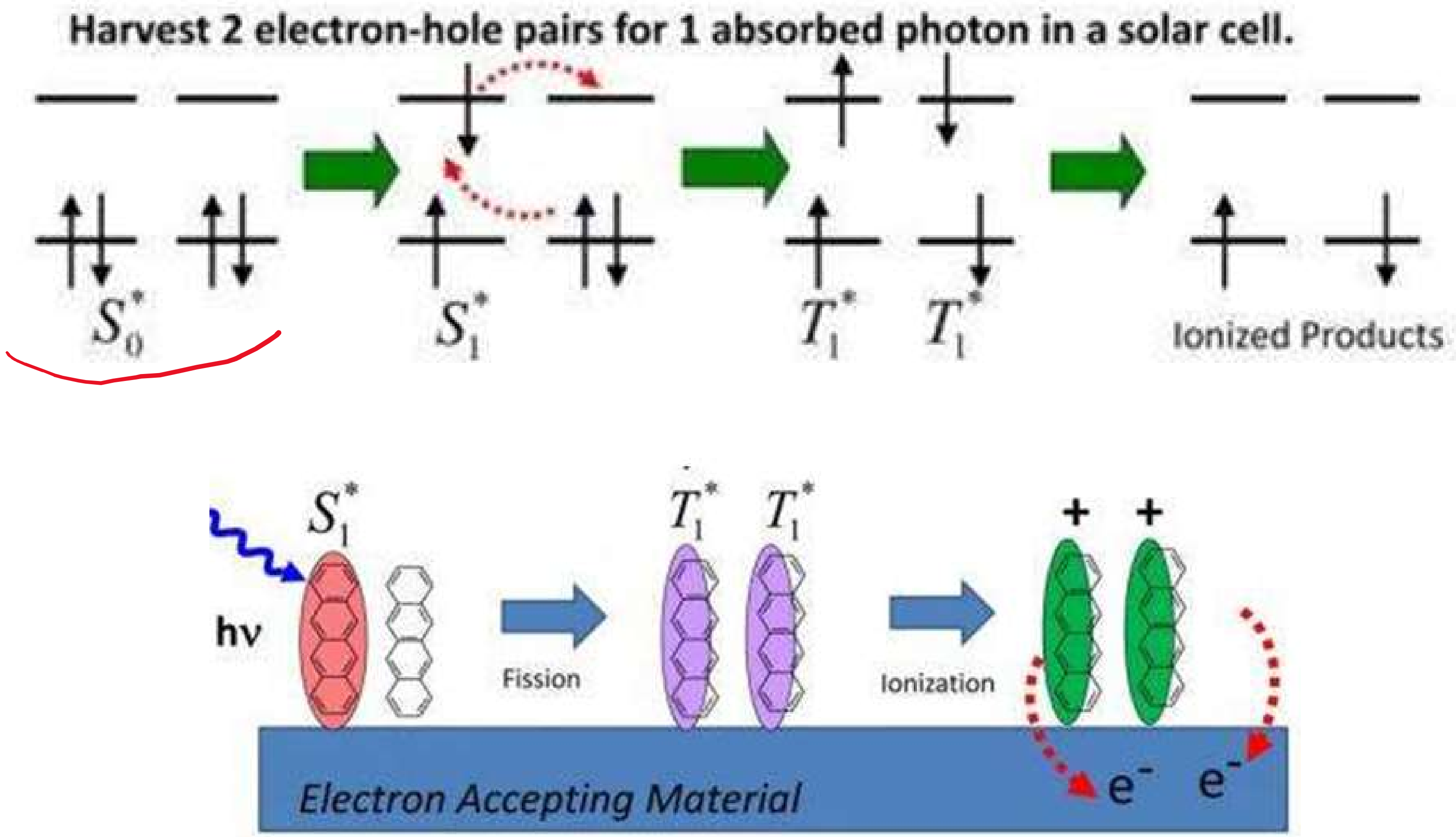


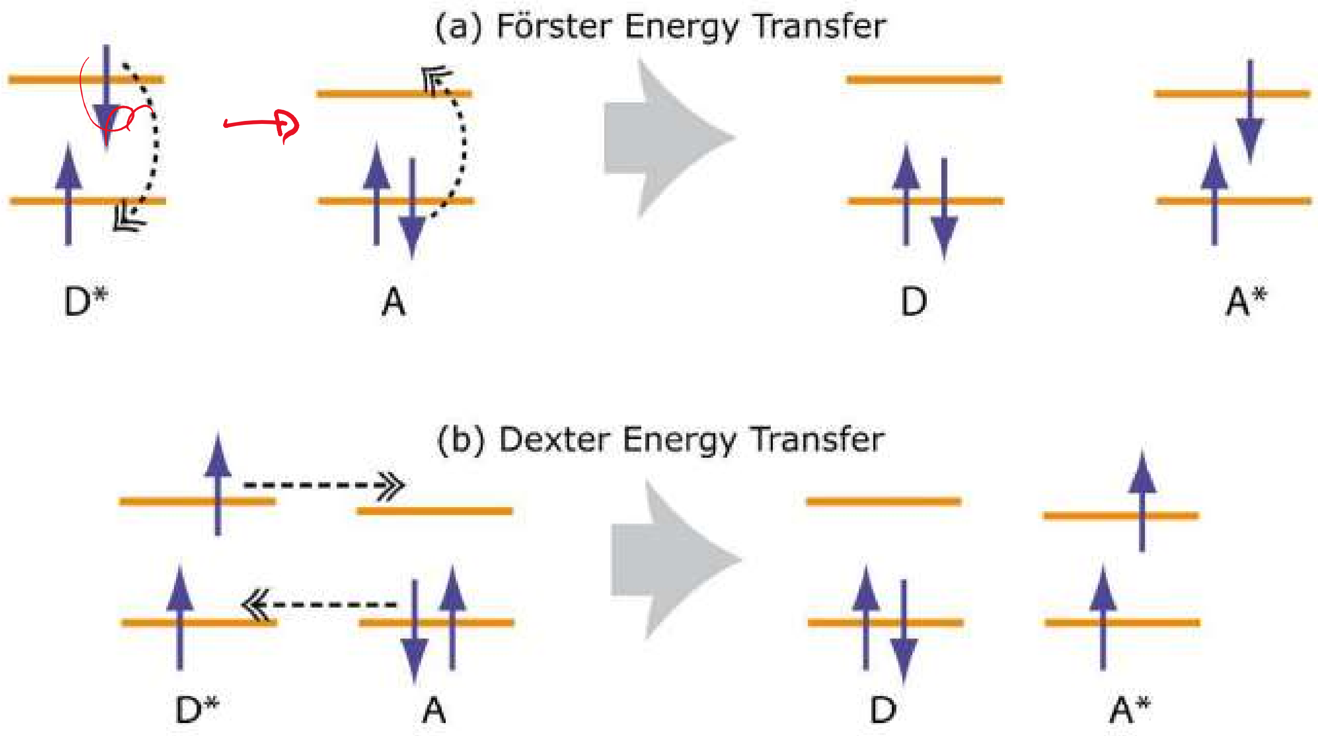




***Energy Environ. Sci.***, 2014,**7**, 499-512

# Singlet Fission




*J. Phys. Chem. Lett.* 2014, 5, 13, 2312–2319




***Energy Environ. Sci.***, 2015,**8**, 1867-1888

$h\nu_1 \rightarrow$ crea l'eccitone ($S_1$)

$\Delta t$ delay pump-probe

$h\nu_2 \rightarrow$ fotoemissione