FACULTÉ DES SCIENCES ET TECHNOLOGIES
Département Physique

Université de Lille

Advanced Characterization Methods II : Radiation interactions with matter

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Outline

1- Introduction

Particles and interactions

Particles that are used for characterization
- Photons
- Electrons
- Neutrons
- Ions

2 types of interactions
- Elastic interaction: no energy transfer
- Inelastic interaction: energy transfer

Energy transfer depends on
- The nature of the interaction
- The interaction mechanism
- Frequency and probability of the interaction

Measurement families

Diffraction
- Atoms organized in space
  → incoming radiation will be scattered in some specific direction
  → study of organization of the scattered radiation will provide input on atom layout in space

Spectroscopy
- Atoms or structures absorb part of the incoming radiation and emit other radiations
  → study of the absorption / scattering energies
  → information on chemistry, vibrations, etc

Microscopy
- The interaction depends on location in the sample
  → formation of 2D or 3D images

2- Electronic structures

Atomic electronic structure

Atom with atomic number Z

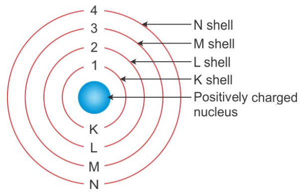
- Positive charge in the nucleus Ze (Z protons and some neutrons)
- Electron cloud with charge -Ze

Shrödinger equation, quantum mechanics

- Electrons are placed at quantified energy levels, shells and subshells
- Quantum numbers n, l, m, s

Pauli exclusion principle

- 2 electrons can not be in the sample



Electron shells

- n=1 (K), max 2 e^-
- n=2 (L), max 8 e^-
- n=3 (M), max 18 e^-
- n=4 (N), max 32 e^-
- n=5 (O), max 50 e^-
- etc

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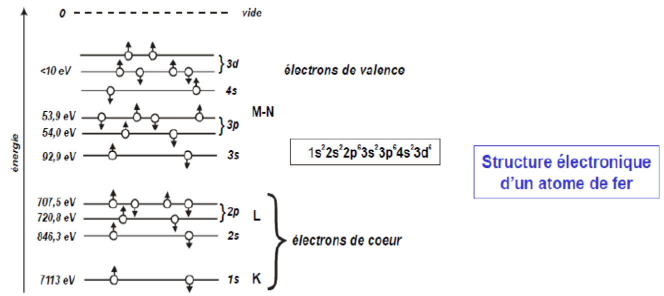
Illustration: iron electronic structure



Energy scale:
energy required to eject the electron from the atom

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3- General concepts

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Incoming radiation

I : intensity = number of particles per time unit

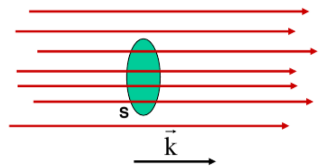
F : flux = number of particles per time and surface unit

E : incoming particles energy

k : wave vector

- Direction of the incoming flux
- Norm proportional to energy

temps t :
n particules
I=n/t
F=I/S=n/(tS)



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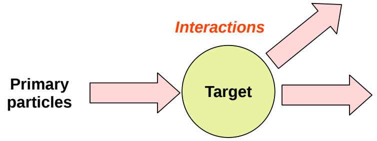
Interaction with target

Scattering (change in *k*)

- **Coherent (without energy loss)**
- **Incoherent (with energy loss)**



Transmission (no change in *k*)

- **Energy loss**
- **Absorption (decrease of I)**

Effects on target

- Local heating (meV)
- Excitation of vibrations and rotations (vibrons, rotons) (1-100 meV)
- Elastic waves (phonons, plasmons) (1-10 eV)
- Excitation of external electronic levels (1-100 eV)
- Excitation of core electronic levels (100 eV – 100 keV)
- Atomic displacement
- Etc

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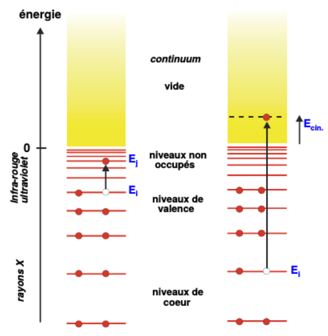
Excitation vs. ionization

Excitation

- Electron transfer to a higher energy level
- No charge change for the atom
- Energy given to the electron = energy difference between both levels

Ionization

- Ejection of the electron
- Charge change for the atom
- Energy given to the electron > ionization energy



Excitation
$\Delta E = E_j - E_i$

Ionisation
$\Delta E = E_c + E_i$

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4- Interactions of photons with matter

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Photon energy

Infrared
- 1 mm to 0.7 µm
- 10^{-3} to 1 eV

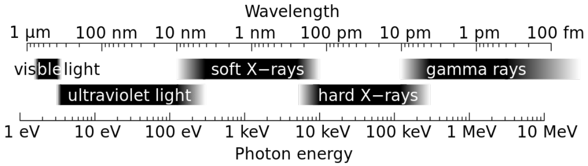
Visible light
- 400 to 700 nm
- 1 to 3 eV

Ultraviolet
- 10 nm to 400 nm
- 3 to 100 eV

Soft-X-rays
- 0.1 nm to 10 nm
- 100 eV to 10 keV

Hard-X-rays
- 0.005 to 0.2 nm (0.05 to 2 Å)
- 5 to 300 keV

Gamma-rays
- E > 100 keV



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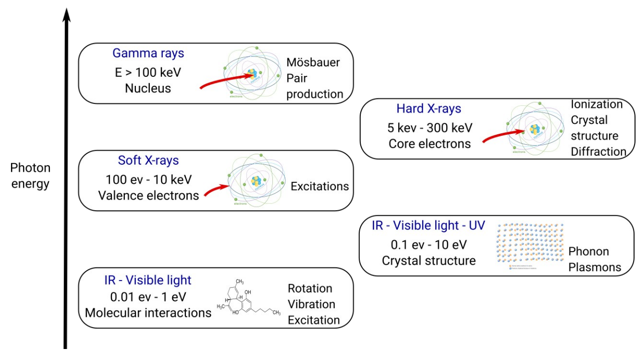
Effect of photon energy



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Photon-matter interactions

Atomic scale
- Thomson – Rayleigh diffusion
- Photo-electric effect
- Compton effect
- (materialization and nuclear reactions; high energy)

Crystalline scale (low energy)
- Molecular interactions (vibrations, rotations, etc)
- Phonons (collectives oscillations of atoms)
- Plasmons (collectives oscillations of electrons)

Crystalline scale (high energy)
- Diffraction

Incoming photon parameters
- Intensity I_0
- Wavelength / frequency λ_0 / ν_0
- Wave vector $\mathbf{k}_0$
- Energy $E_0 = h\nu_0$

After the interaction
- Transmission
  - Less intensity (absorption) $I < I_0$
  - Energy loss $E < E_0$, transmitted energy spectrum $I(E)$
- Change of wavevector **k**: scattering
  - No energy loss: elastic scattering
  - With energy loss: inelastic scattering

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4.1- Interactions of photons with matter Atomic scale

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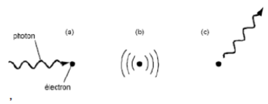
Thomson/ Rayleigh scattering

Low energy photons (IR, visible)
Photon absorbed and re-emitted in another direction → scattering
No change in energy → elastic scattering

Thomson scattering
- Photon absorbed by a single electron
- Excited state for the electron
- Emission of a new photon, same E, but ≠ direction



Rayleight scattering
- Photon interacts with the whole electron cloud
- Excited state
- Emission of a new photon, same E, but ≠ direction

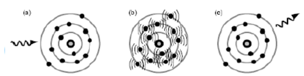


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Photo-electric effect (50 eV – 50 keV)

Interaction between a photon and electrons

- Incoming photon E = h ν
- Ionization and absorption of the photon
- Kinetic energy of the electron
  $E_c = h\nu - E_i$
- Excited electronic state in the atom
- Emission of multiple X-ray photons to return to the atomic ground state

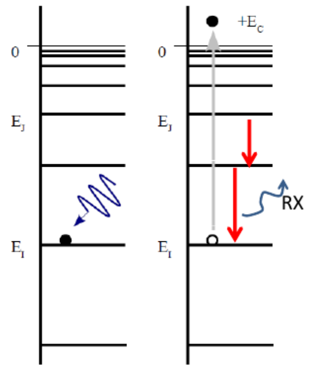

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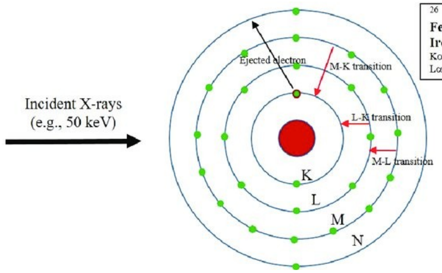
Illustration : Iron



Kα (K-alpha) :
- L to K transition
- Emission of a photon with 6.4 keV

Kβ (K-beta) :
- M to K transition
- Emission of a photon with 7.1 keV

Lα (L-alpha) :
- M to L transition
- Emission of a photon with 0.7 keV

Illustration : Teixeira Ribeiro, Ciência e Agrotecnologia, 2017

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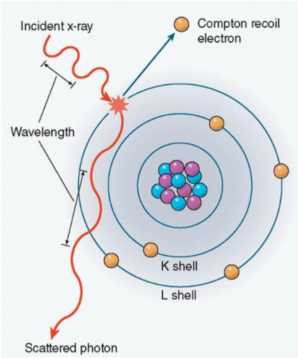
Compton scattering

Interaction between incoming photon and electrons in the electron cloud

Ionization + creation of a new photon

Energy conservation:
incoming photon energy =
scattered photon energy +
scattered electron energy +
ionization energy



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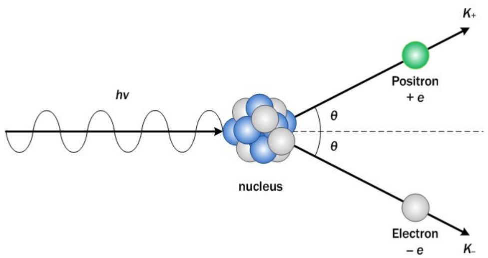
Pair production



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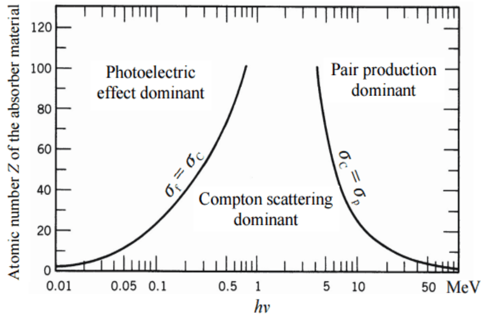
Effect of atomic number and photon energy



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Atom – photon interactions: summary

Thomson-Rayleigh scattering

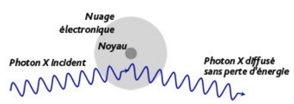
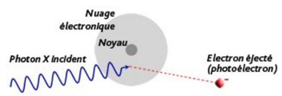
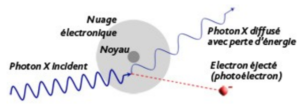


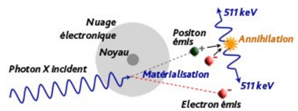
Photo-electric effect



Compton scattering



Pair creation



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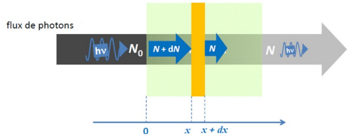
Attenuation

X-ray absorption by matter



$$N = N_0 e^{-\mu x}$$

N : number or flux of photons

x : sample thickness

μ : linear attenuation coefficient

Table on side: 50% attenuation length, L = ln(2)/μ

ordre de grandeur *CDA*: CDA = couche de demi-atténuation

	30 keV	100 keV	500 keV
air	25 m	35 m	60 m
eau (*liquide*)	2 cm	4 cm	7 cm
béton	3 mm	2 cm	4 cm
plomb	0,02 mm	0,1 mm	4 mm

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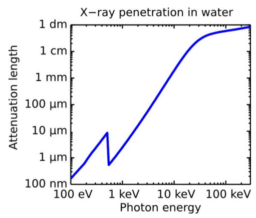
Attenuation

Attenuation is an effect of the different scattering mechanisms

Linear attenuation coefficient μ depends on

- Material composition
- Photon energy



Attenuation length in water

- E = 100 eV (λ ~ 120 Å) : ~ 100 nm
- E = 30 keV (λ ~ 0.5 Å) : ~ 10 cm

Peak at 930 eV

- Ionisation E of oxygen (threshold for photo-electric effect)
- Possible above 930 eV → absorption increases at 930 eV

Saturation at 20 keV

- Compton effect kicks in

Image wikipedia

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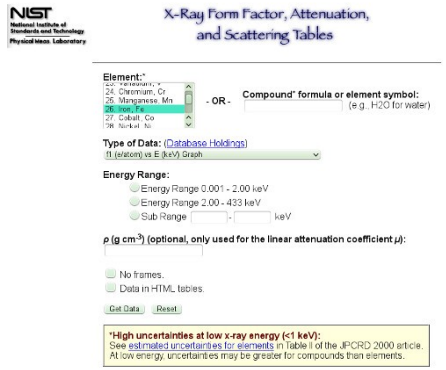
Databases

X-ray scattering databases at NIST (National Institute of Standards) :

- http://physics.nist.gov/PhysRefData/Xcom/html/xcom1.html
- http://physics.nist.gov/PhysRefData/FFast/html/form.html



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Example: mass attenuation coefficient for Fe

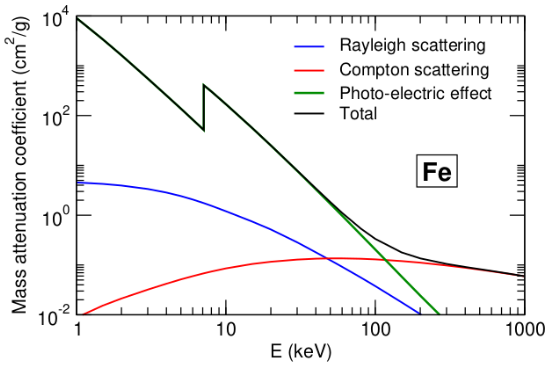

Figure generated from data on the NIST databases

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4.2- Interactions of photons with matter
Crystal and molecular scale

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Vibrons, rotons, phonons, plasmons

Photons can interact with

- vibrons: vibration modes in a molecule or a structure
- rotons: rotation modes in a molecule or a structure
- phonons: collective oscillations of atomic cores, acoustic waves in a solid
- plasmons : collective oscillations of atom electrons

Spectroscopy techniques : infra-red, Raman, Brillouin, etc

More details in Advanced Characterization I

Remember that it works on solids as well

Many possibilities for photons / molecules interactions

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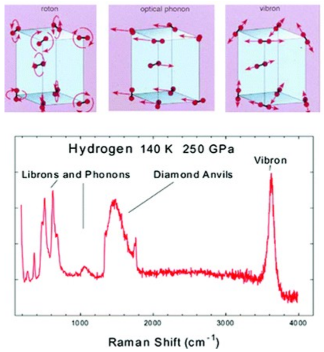
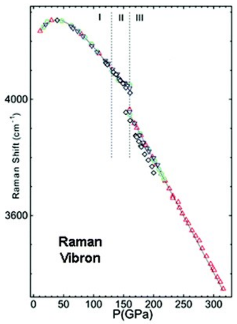
Example: Solid H_2 – 140 K – 250 GPa





Goncharov and Hemley, *Chem. Soc. Rev.*, 2006, **35**, 899-907

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Diffraction

Cf next class

X-rays diffraction

- Effect on electronic cloud
- Rayleigh scattering by the electronic cloud
- Constructive interference between scattered photons

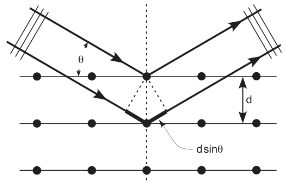
$$n\,\lambda = 2\,d_{hkl}\,\sin\theta$$

λ : incident wavelength

d_{hkl} : distance between 2 crystal plane families

θ : Bragg angle

n : order of diffraction (integer)



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5- Interactions of electrons with matter

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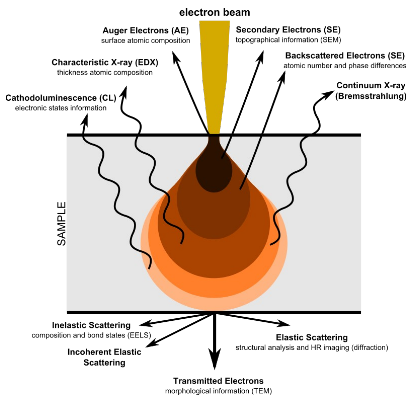
Electron-matter interactions: a summary



SEM mostly use thick samples → no signal in transmission

TEM use thin samples → can work on both transmission and reflexion

Illustration Wikipedia

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Electron-matter interactions

Elastic scattering by the atomic potentials

- Far from the atom

Inelastic scattering by electrons of the electronic cloud

- Within the atomic radius

Deceleration radiation in the material

- Close to the atomic core

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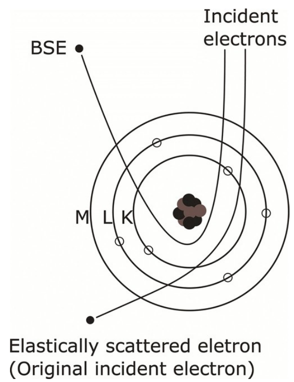
Electron elastic scattering



Coulomb forces between the incoming electron, the nucleus and the electronic cloud.

Most efficient for atoms with a high Z number

Forward scattering (that goes through the sample) is used to create diffraction images in the TEM.

Backwards scattering is used for imaging in the SEM.

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Inelastic scattering

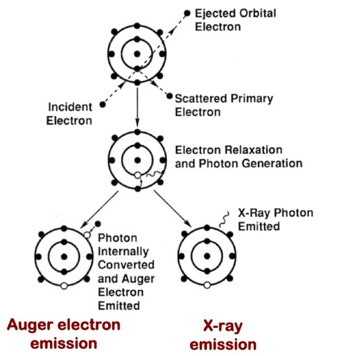
Incoming electron, interaction with electron in the electron cloud
→ scattered electron + ejected electron

Ejected electron = secondary electron

Relaxation of electronic cloud
→ photon emission

Photon can be emitted directly, typically in the X-rays
→ X-ray emission

Photon can be absorbed by the atom, with emission of another electron
→ Auger electrons



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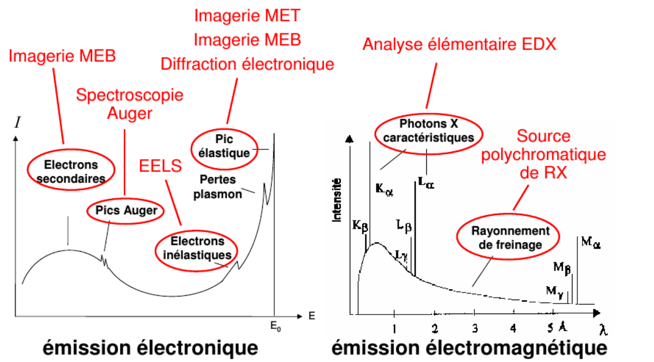
Electron-matter interactions: emission spectrum



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Mode details

Classes of Damien Jacob on electron microscopy

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6- Interactions of neutrons with matter

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Generalities on neutrons

“heavy” particles with no charge

- Nearly no interaction with electrons
- Interactions with the nucleus

Interaction depends on

- The target nucleus
- Incoming neutron energy

Classification of neutrons

- Slow (thermal) neutrons : $E_n < 0.5$ eV
- Intermediate neutrons: 0.5 eV $< E_n <$ 10 keV
- Fast neutrons: $E_n >$ 10 keV

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Possible neutron matter interactions

Elastic scattering

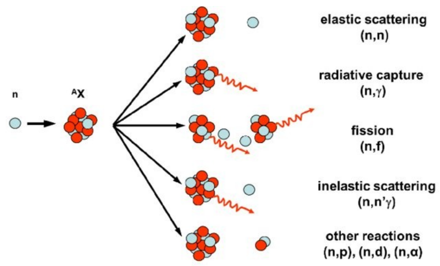
- No change in the target atom
- Some of the incoming energy transferred to the target

Inelastic scatting

- Emission of photons
- No change in the target atom
- Some of the incoming energy transferred to the target

Nuclear reactions

- Changes in the target atom



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Extra

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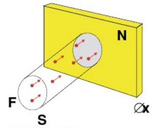
Section efficace

Section efficace : caractérise l'efficacité d'une interaction

flux incident — *nombre d'atomes par unité de volume*

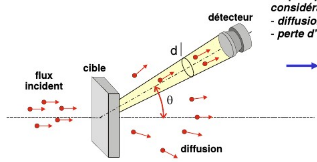
nombre d'interactions → $dn = F.N.\sigma.S.\varnothing x = I.N.\sigma.\varnothing x$

section efficace totale



en cm² ou en barn (10^{-24} cm²)

On peut particulariser l'interaction en ne considérant qu'une fraction de l'évènement :
- diffusion dans une direction donnée
- perte d'une quantité précise d'énergie…



→ section efficace différentielle

$$\sigma(\theta) = \frac{d\sigma}{d\theta}$$

$$\sigma = \int \frac{d\sigma}{d\theta} d\theta$$

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