

A Rapid Photoemission Model for Beam Optics Codes



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Abstract

Photocathodes for future Vacuum Electronic (VE) applications such as x-ray Free Electron Lasers (xFELs) and particle accelerators must satisfy metrics related to performance addressing: (i) the mean transverse energy of the beam, (ii) the effects of surface roughness, (iii) the nature and dependencies (e.g., temperature) of scattering processes, (iv) the impact of non-uniform coverage of coatings, (v) the dependence on temperature, (vi) how degradation and damage due to dark current, desorption, and back-ion bombardment occur, and (vii) the dependence on the composition (aka stoichiometry) of the photoemissive material. Beam optics codes used to design VE devices launch macroparticles from millions of surface elements for millions of time steps, and so prioritize algorithmic simplicity and rapidity of execution. We present a high speed and flexible algorithm that gives QE based on the parameterization of the dielectric function $K(\omega)$ using Lorentz-Drude-Resonant (metal, m) and Adachi-Drude-Resonant (semiconductor, s) schemes, and show how Nordheim's alloy scattering rule and Drude's model of conductivity allow composition to affect estimates of (E_g, E_v, r_e) for band gap, electron affinity, effective electron mass, that appear in the QE Formulae (see (14), (15), (20) and (21)). It is therefore expected that composition will change these most important factors on which QE depends. We demonstrate the model's speed and performance as applied to measured QE from copper and Cs_3Sb and consequences of stoichiometric variation of the later.

UNITS AND NOTATION: I

"Though this be madness, yet there is a method in't."
W. Shakespeare, *Hamlet*, II.ii.203-204

Fundamental Constants

Symbol	Definition	Value
q	unit charge	q
$\hbar$	Planck Const.	0.658212 eV·fs
c	speed of light	299.792 nm/fs
m	e^- rest mass	510999 eV/ c^2
k_B	Boltzmann	1/11604.5 eV/K
a_0	Bohr Radius	0.052918 nm
α	Fine Struc.	1/137.036
Q	$\alpha\hbar c/4$	0.36 eV·nm
$Q/2a_0$	Rydberg Eng.	13.606 eV

Establish units and notational conventions for what follows

UNITS AND NOTATION: II

Introduce the barrier to electron emission that will be used for the remainder of the Poster

- Schottky Nordheim (Image Charge) Barrier

$$V(x) = \mu + \Phi - q\mathcal{E}x - \frac{q^2}{16\pi\epsilon_0 x} \quad (1)$$

$$\equiv V_o - Fx - \frac{Q}{x}$$

- Schottky Barrier Lowering: $\phi = \Phi - \Delta\Phi$

$$\partial_x V(x_o) = 0 \Leftrightarrow x_o = \sqrt{Q/F} \quad (2)$$

$$\phi \equiv \Phi - \sqrt{4QF} \quad (3)$$

- Sommerfeld Metal & Fermi-Dirac Dist. for evaluation of Supply Function

$$f_{FD}(E_k) = \frac{1}{1 + \exp[(E_k - \mu)/k_B T]} \quad (4)$$

Terms

- μ is Fermi level; Φ is Work Function
- F is a force; V is an energy
"Field" denotes terms dependent upon F
- Dimensionless ratio:
 $y(E) = \frac{V_o - V(x_o)}{\mu + \Phi}; \quad y(\mu) = \frac{\sqrt{4QF}}{\Phi}$
- $\alpha = \frac{q^2}{4\pi\epsilon_0\hbar c} \Leftrightarrow Q = \frac{1}{4}\alpha\hbar c$
- Units of electron emission:
Here: [nefq] = nm, eV, fs, q = 1

General Thermal Field Photoemission Equation I

General Thermal-Field-Photoemission Eq. generalizes the Fowler-DuBridge formula for Quantum Efficiency

Thermal-Field: $n \equiv \beta_T / \beta_F(E_m)$

$$J(F, T) = A_{RLD} T^2 N(n, s) = J_F + J_T$$

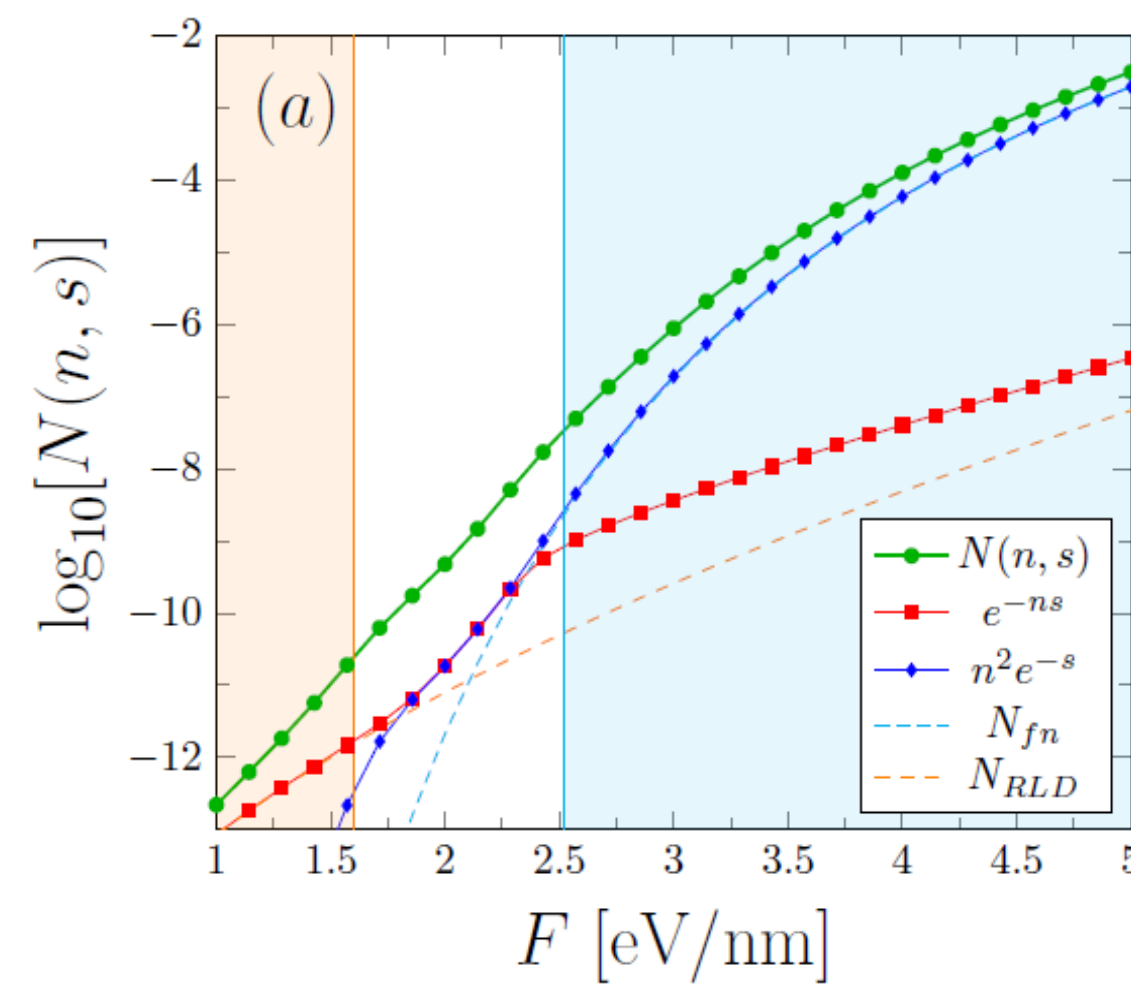
$$N(n, s) \approx n^2 e^{-s} \sum \left(\frac{1}{n} \right) + e^{-ns} \sum (n) \quad (5)$$

$$\Sigma(x) \approx \frac{1+x^2}{1-x^2} - 0.36x^2 - 0.106x^4$$

Photoemission: $E \rightarrow E + \hbar\omega, s \rightarrow -s$

$$N(n, s) + N(n, -s) = \frac{(ns)^2}{2} + \frac{(n\pi)^2}{6}$$

$$J_P \propto (\hbar\omega - \phi)^2 + \frac{\pi^2}{3} \left(\frac{1}{\beta_T^2} + \frac{1}{\beta_F^2} \right) \quad (6)$$

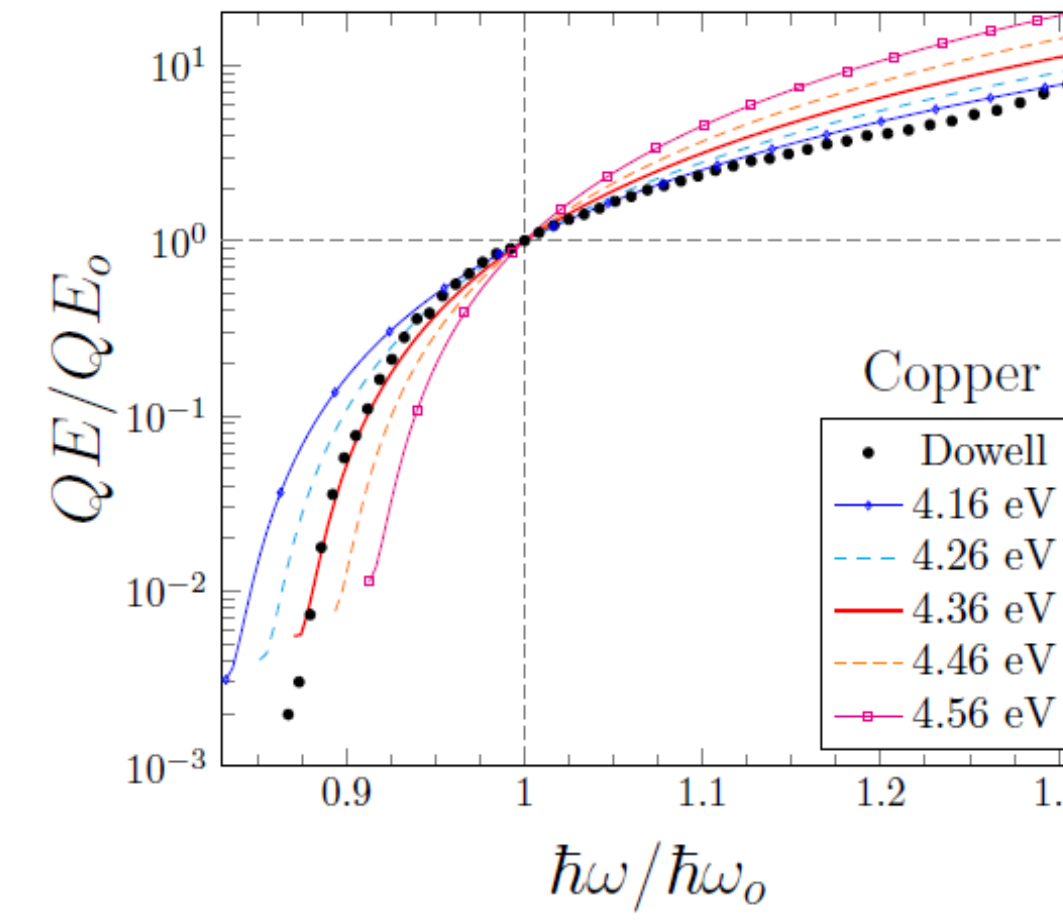


TF Emission: Metal-like parameters
 $\mu = 7$ eV, $\Phi = 4.5$ eV, and $T = 1273$ K

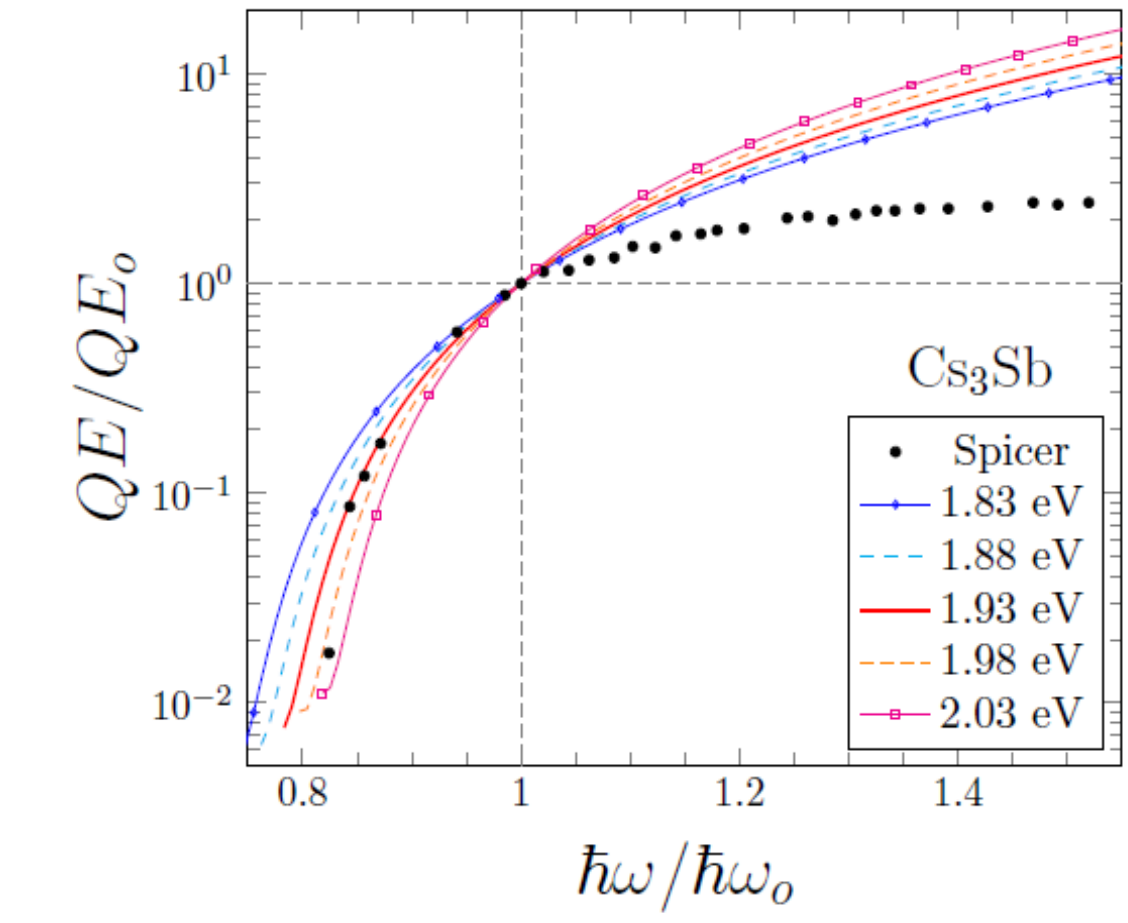
General Thermal Field Photoemission Equation II

Performance of Eq. (6)

Best for threshold emission



$$QE_R(\omega) = QE_{exp}(\omega_o) \left[\frac{(\hbar\omega - \phi)^2 + 2\zeta(2)k_B T^2}{(\hbar\omega_o - \phi)^2 + 2\zeta(2)k_B T^2} \right] \quad (7)$$



PHOTOEMISSION I

Introduce Moments Model (like 3-Step Model) of Quantum Efficiency for PIC Codes

Moments defined by DOS, Absorption, Transport, Emission, & Occupation (metals shown)

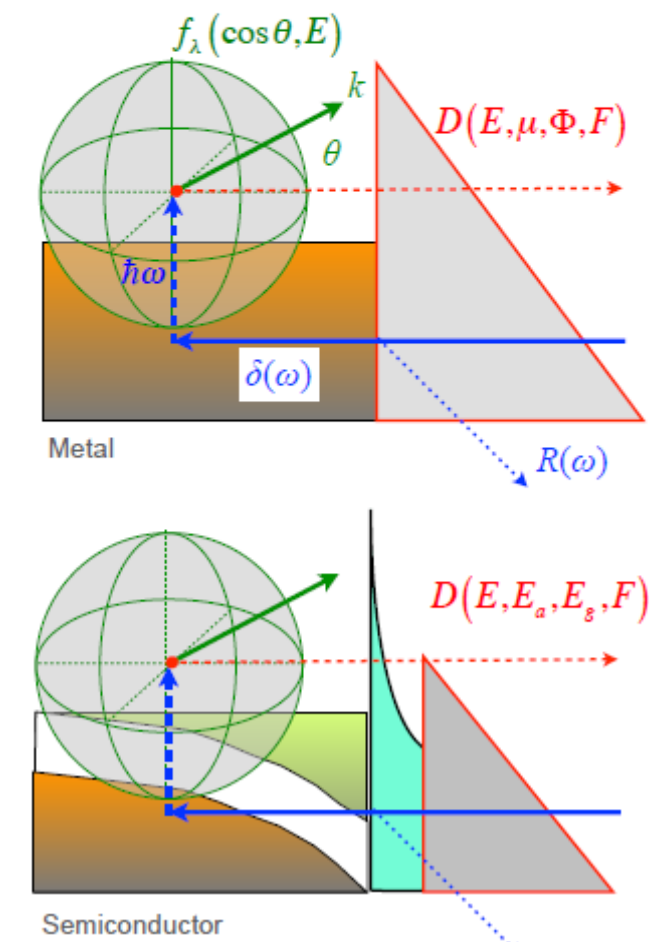
$$M_n(k_z) = \frac{1}{(2\pi)^2} \int_0^\infty \mathcal{D}(E) dE \int_0^\pi \sin \theta d\theta (k \cos \theta)^n f_A(\cos \theta, \vec{E}) D(E \cos^2 \theta) f_{FD}(E) (1 - f_{FD}(\vec{E})) \quad (8)$$

- $\vec{E} = E + \hbar\omega$, $\mathcal{D}(E)$ = density of states, f_A = scattering losses
 $f_{FD}(E)$ initial/final occupation, $D(E_x)$ = step function trans. prob.
- Metals: $x_m = [(\mu + \phi)/(E + \hbar\omega)]^{1/2}$, $s = \cos \theta$

$$QE = \frac{[1 - R(\omega)]}{\hbar\omega(2\mu - \hbar\omega)} \int_{\mu+\phi-\hbar\omega}^\mu E dE \int_{x_m}^1 s ds f_A(s, E) D(Es^2) \quad (9)$$

- Semiconductors: E_g, E_a = band gap, e^- affinity, $s = \cos \theta$, $R(\omega)$ = reflectivity

$$QE = \frac{[1 - R(\omega)]}{(\hbar\omega - E_g)^2} \int_{E_a}^{\hbar\omega - E_g} E dE \int_{\sqrt{E_a/E}}^1 s ds f_A(s, E) D(Es^2) \quad (10)$$



PHOTOEMISSION II

- Metals: losses dominated by $e-e$ scattering which rapidly reduces KE: short mean free path
- Semiconductors: magic window where $e-e$ scattering forbidden and only $e-p$ (small energy loss) occurs: long mean free path
- Fatal Approximation: Assume ANY scattering prevents (is fatal to) emission:
 - δ : how far laser light gets in
 - $x/\cos \theta$: how far e^- go to get out
 - $\ell(E) = v(E)r(E)$: mean free path
- dimensionless ratio $p(E) = \delta(\omega)/\ell(E)$

Emission part of Moments model: Conveniently separate out the transmission over / thru barrier part of the QE integral

Metals

$$h_m(s, r) = \frac{(s-1)(3r-s+1)}{6s(2r-s)} \quad (12)$$

Semiconductors

$$h_s(s) = \frac{s^5}{u^2(1+u)(s+u)^2} \quad (13)$$

$$u^2 = 1 + s^2$$

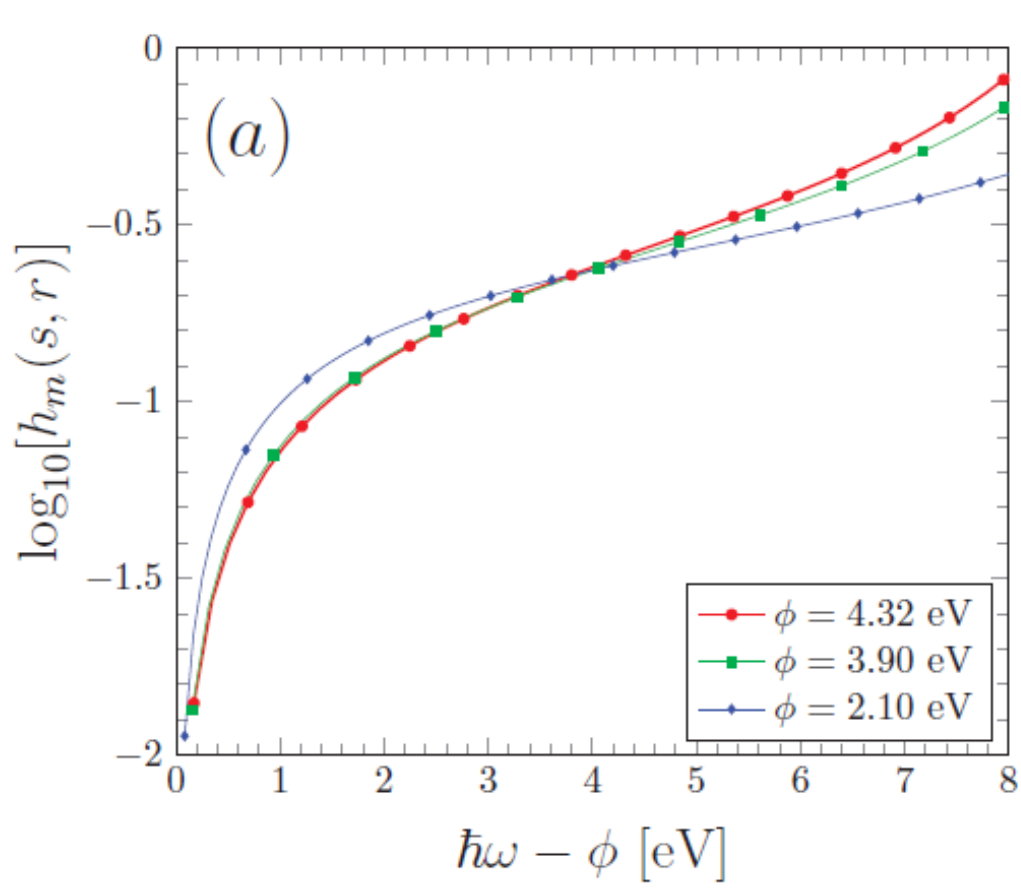
$$f_A(\cos \theta, p) = \frac{\cos \theta}{\cos \theta + p(E)} \quad (11)$$

$$F_A(x_m, E) \equiv \int_{x_m}^1 D(Ey^2) f_A(y, E) y dy$$

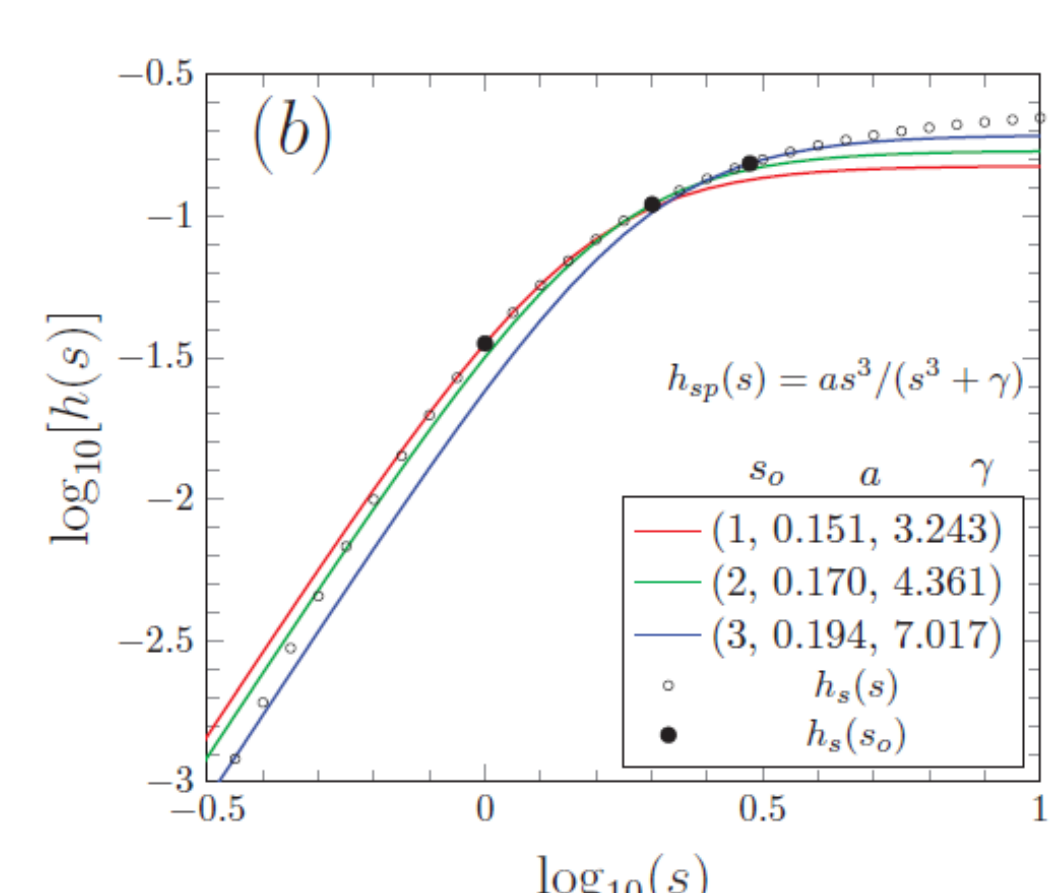
PHOTOEMISSION III

Jensen, Dimitrov, Finkenstadt, Wang, Pavlenko, Aryal, Batista, Petillo, Rocco, O'Shea, JAP139, (2026). DOI: 10.1063/5.0331812

$$QE_{metal} \approx [1 - R(\omega)] F_A[x_m, p] h_m \left[\frac{\hbar\omega}{\phi}, \frac{\mu}{\phi} \right] \quad (14)$$



$$QE_{semi} \approx \left[\frac{1 - R(\omega)}{1 + p} \right] h_s \left[\sqrt{\frac{\hbar\omega - E_g - E_a}{E_a}} \right] \quad (15)$$



LDR / ADR OPTICAL MODEL I

For PIC, represent Dielectric Function as a sum over Lorentzians to enable rapid computation, flexibility in modeling small changes due to material, stoichiometry

- Dielectric const. $\hat{K}$ (Plasma freq: $\omega_p^2 = 16\pi Q\rho_o/m$)
Free (metal-like) and Bound (insulator-like) contributions

$$\hat{K}(\omega) = 1 + \hat{\chi}_f(\omega) + \hat{\chi}_b(\omega) = K_r + iK_i \quad (16)$$

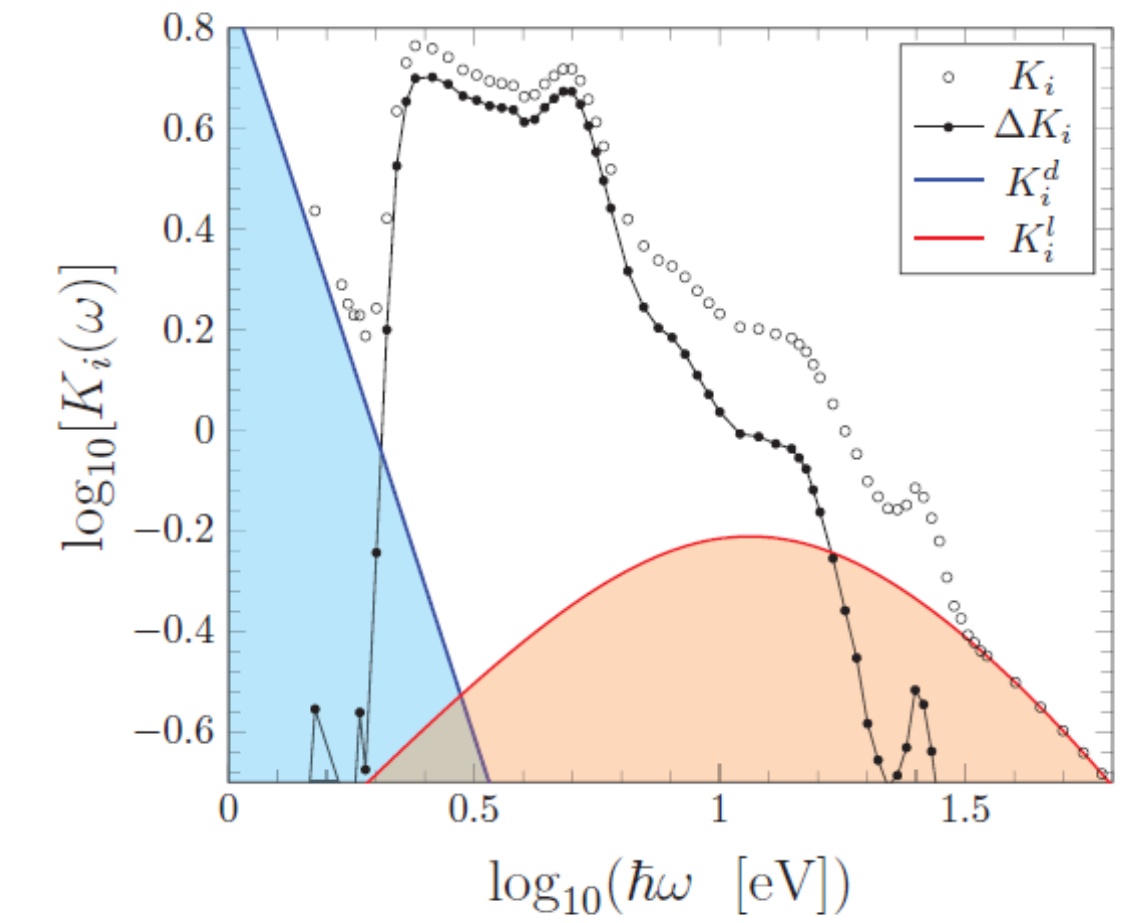
- Drude (ω small) and Lorentz (ω large)

$$\hat{\chi}_d(\omega) = -\frac{f_d \omega_p^2}{\omega(\omega + i\Gamma_d)}, \quad \hat{\chi}_l(\omega) = -\frac{f_l \omega_p^2}{\omega^2 - \omega_l^2 + i\omega\Gamma_l} \quad (17)$$

- Dielectric, Reflection, Penetration

$$2n^2 = |\hat{K}|^2 + K_r, \quad 2k^2 = |\hat{K}|^2 - K_r \quad (18)$$

$$R(\omega) = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}, \quad \delta(\omega) = \frac{c}{2k\omega} \quad (19)$$



Blue: Drude part Red: Lorentz part

LDR / ADR OPTICAL MODEL II

After extracting Drude and Lorentz part (for metals), fit the remaining peaks in K_i with Resonant terms (more Lorentzian)

- LDR (metal): Resonant terms ($(l \rightarrow (j=0))$)

$$\hat{K}(\omega) = 1 + \hat{\chi}_f(\omega) + \hat{\chi}_b(\omega) = K_r + iK_i$$

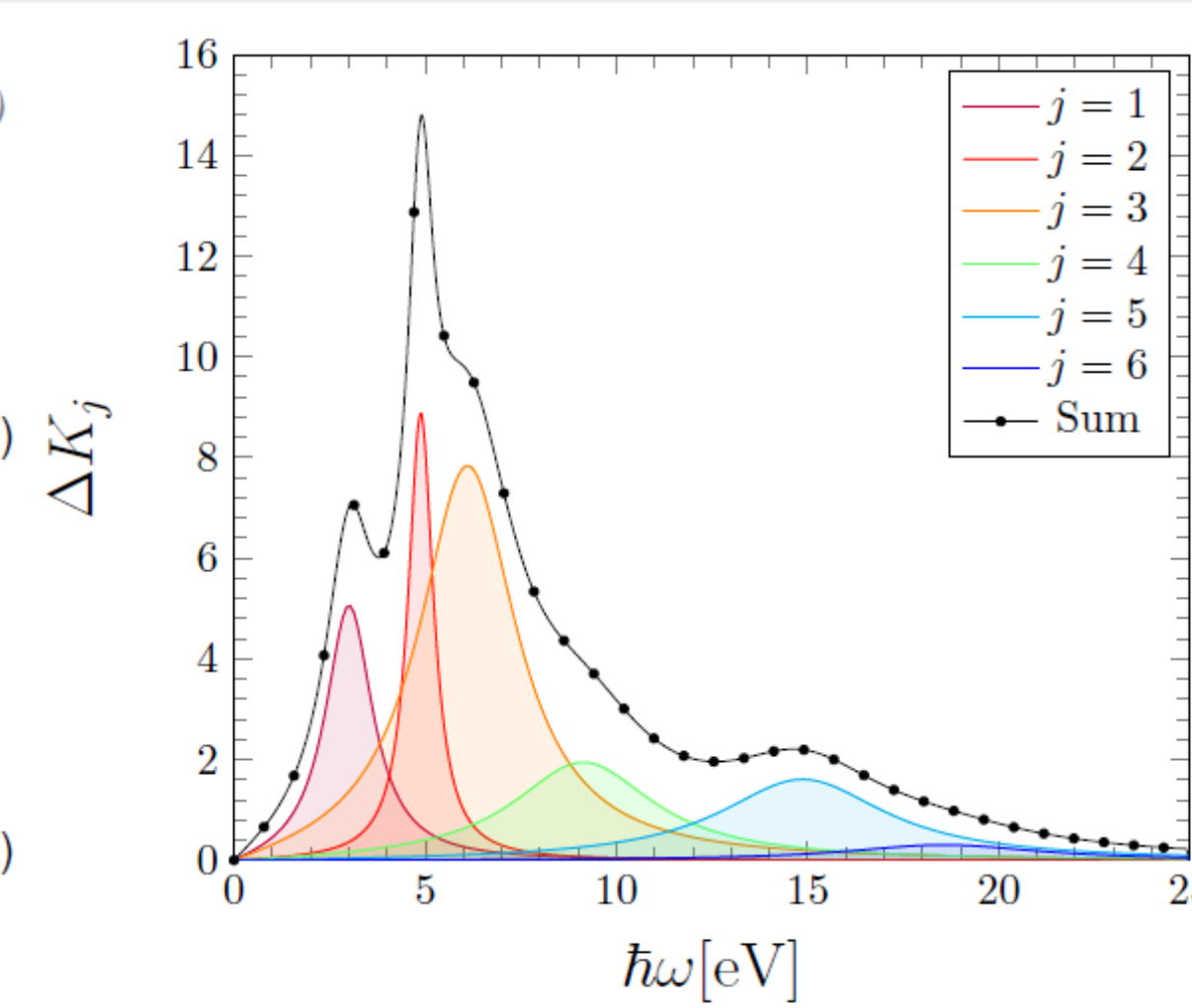
$$\hat{\chi}_f(\omega) = -\frac{f_d \omega_p^2}{\omega(\omega + i\Gamma_d)}$$

$$\hat{\chi}_b(\omega) = -\sum_{j=0}^{N_b} \frac{f_j \omega_p^2}{\omega^2 - \omega_j^2 + i\omega\Gamma_j} \quad (20)$$

- ADR (semiconductor): $\hat{h} = (\hbar\omega + i\eta)/E_g$

$$\hat{K}(\omega) = 1 + \frac{\mathcal{A}}{\hbar p} \left(2 - \sqrt{1 - \hat{h}} - \sqrt{1 + \hat{h}} \right) \quad (21)$$

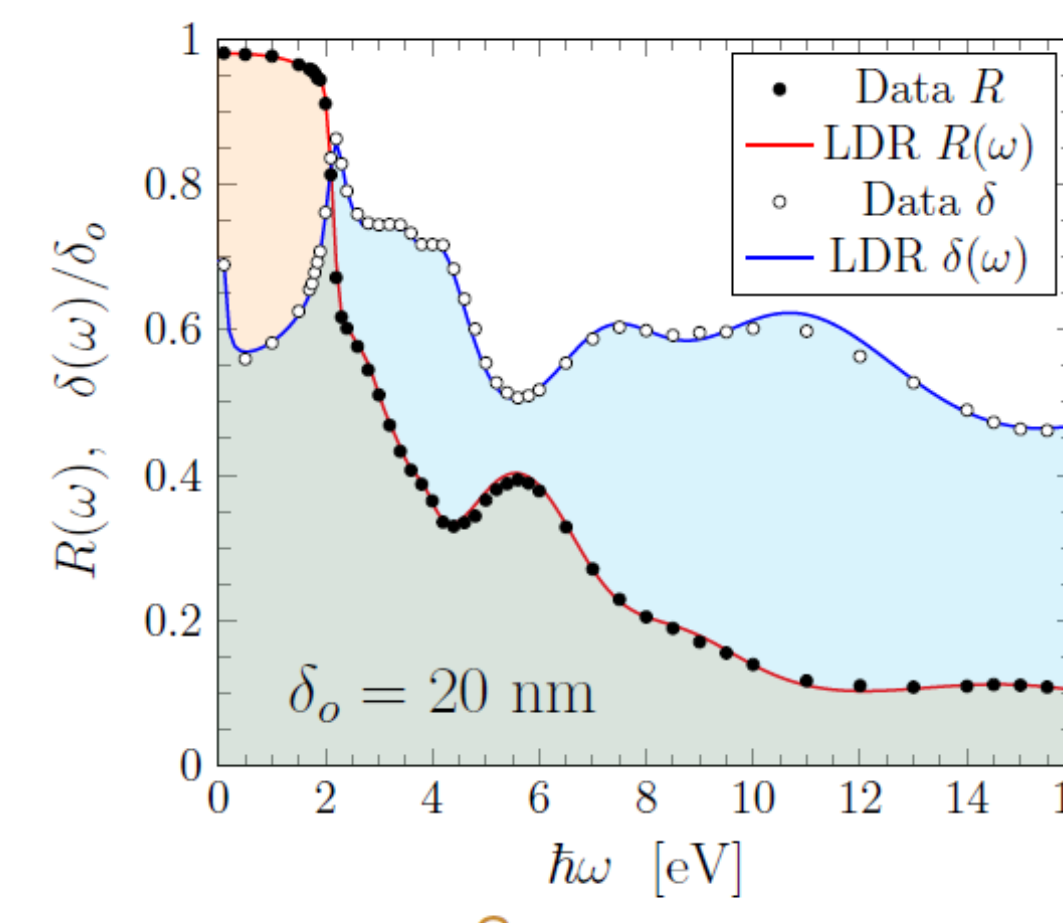
LD / AD combination removed before R components determined



$\Delta K = K_i - K_d - K_l$ (metal) or $= K_i - K_d - K_a$ (semi)
(only imaginary parts used in this eq.)

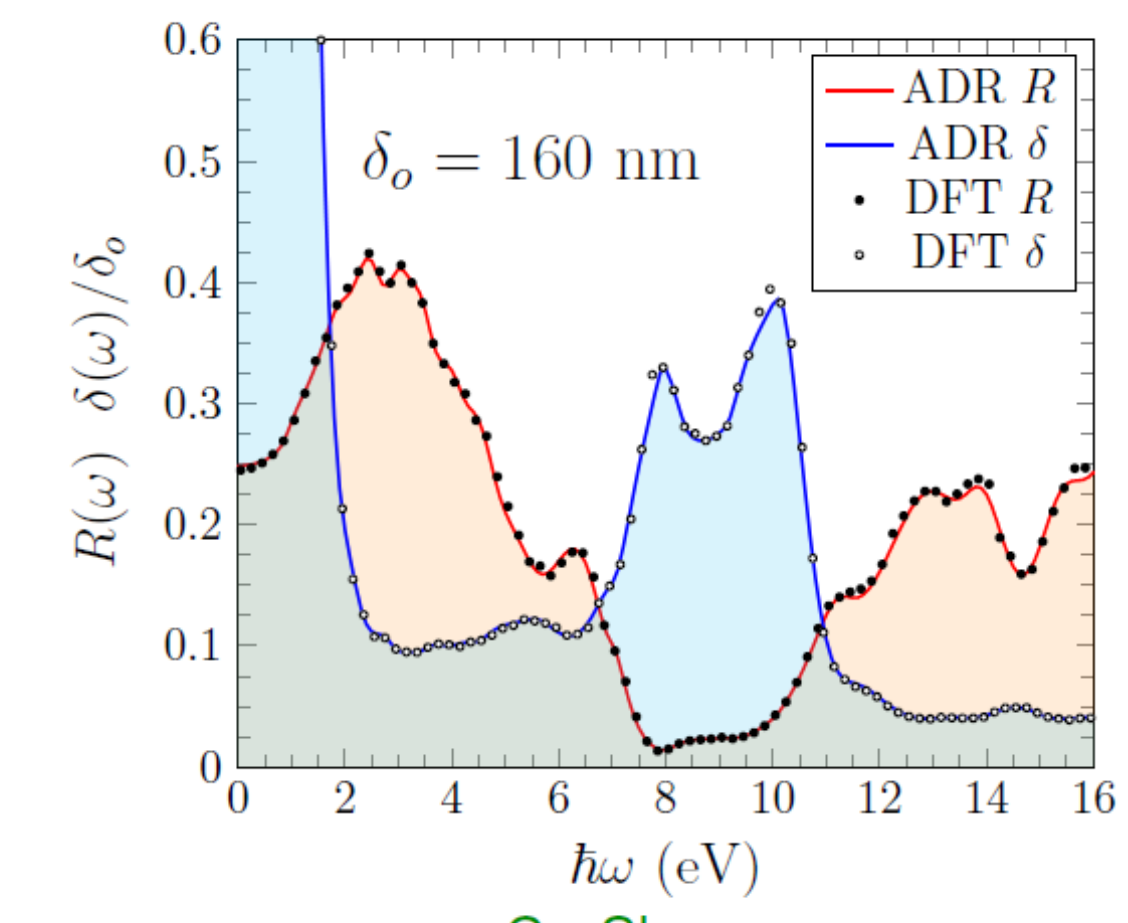
LDR / ADR OPTICAL MODEL III

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Copper

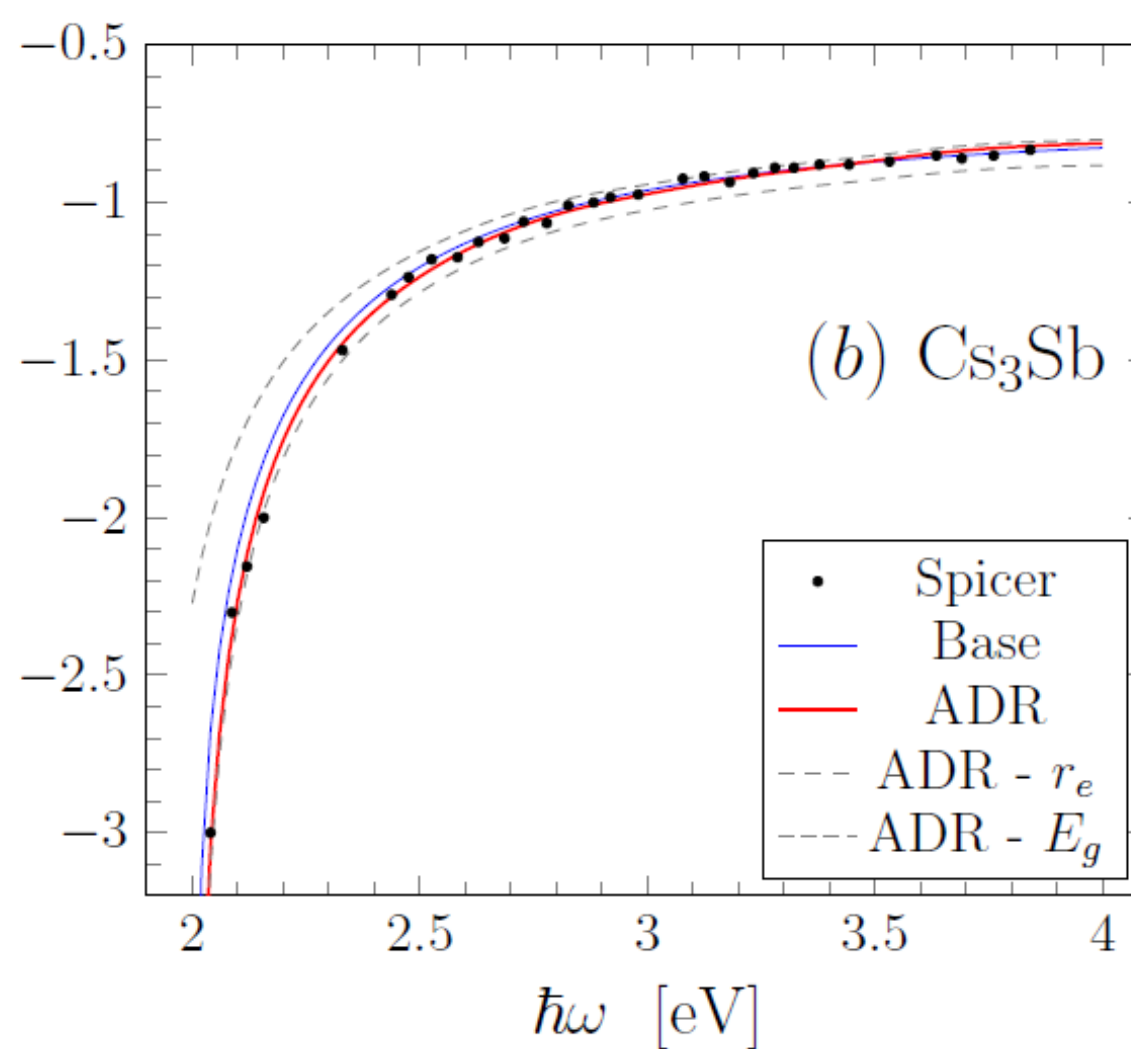
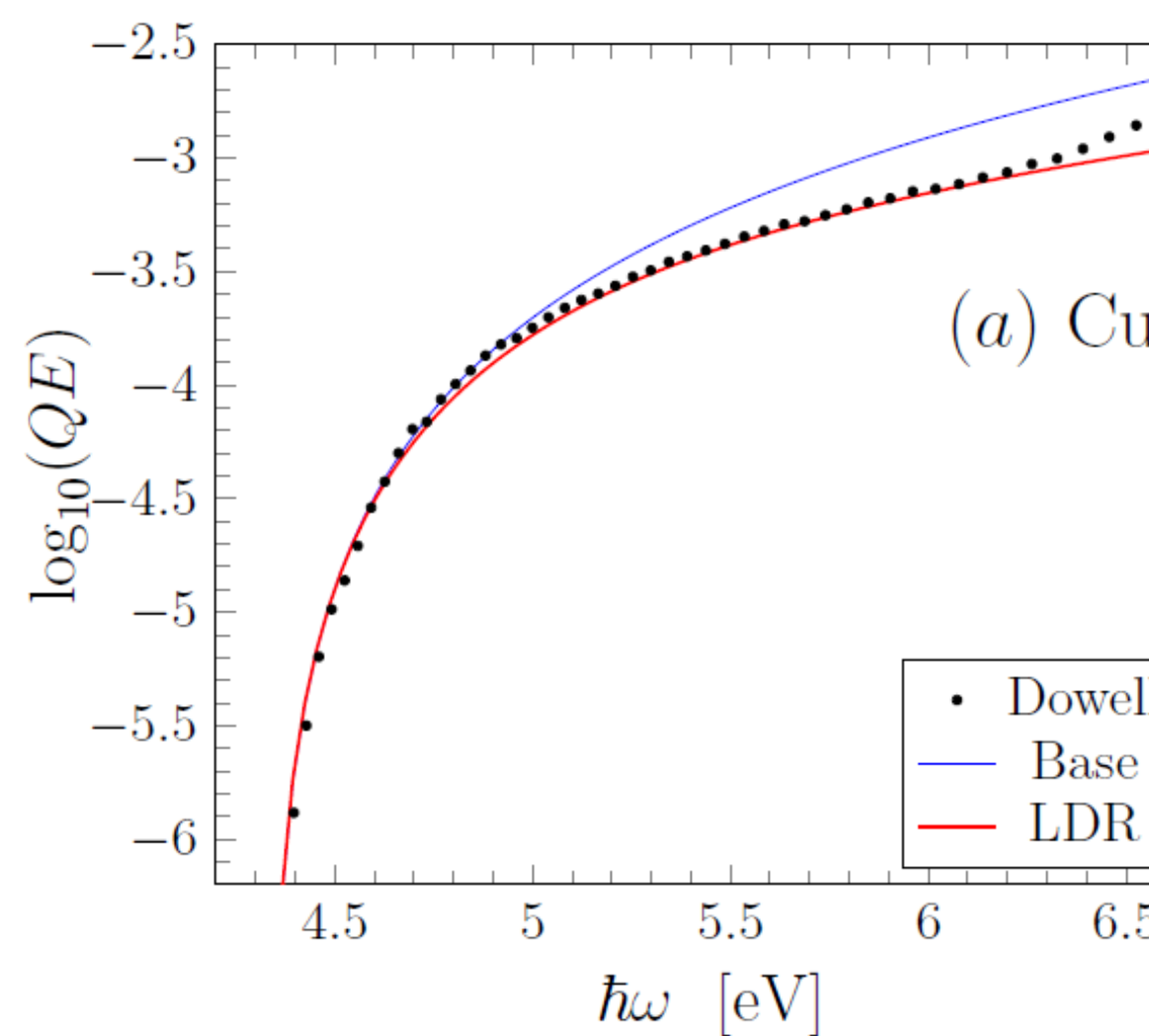
Good and rapid model of reflectivity, laser penetration depth for PIC



Cs3Sb

LDR / ADR OPTICAL MODEL IV

Jensen, Dimitrov, Finkenstadt, Wang, Pavlenko, Aryal, Batista, Petillo, Rocco, O'Shea, JAP139, (2026). DOI: 10.1063/5.0331812
"Base" = Fowler-DuBridge (Cu) and Spicer parametric (Cs_3Sb) models. (r_e, E_g) = effective e^- mass, band gap: both altered by material and stoichiometry



SUMMARY

We have:

- Introduced canonical equations of electron emission
Richardson-Laue-Dushman = thermal; Fowler-Nordheim = field; Fowler-DuBridge = photo
item Introduced Generalized Thermal-Field-Photoemission (GTFP) Eq.
recovers RLD, FN, FD in appropriate limits
- Introduced Moments Model of Quantum Efficiency
- Shown Mods (tunneling, optical) leading to rapid evaluation of QE for PIC

Questions? Please email: kjensen@umd.edu

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