Monte Carlo Study of Photoemission Properties of Semiconductor Cathodes for Accelerator Applications

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Requirements for advanced electron sources

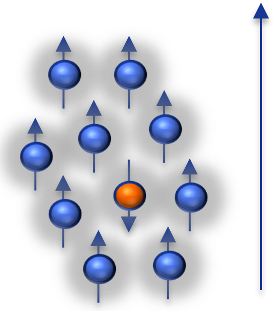
High-quality photocathodes =

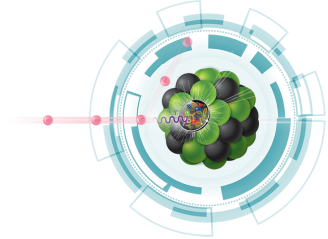
- high quantum efficiency

$$QE = \frac{N_{e^-}}{N_{\hbar w}}$$

- high electron spin polarization (for polarized electron sources)

$$ESP = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}$$

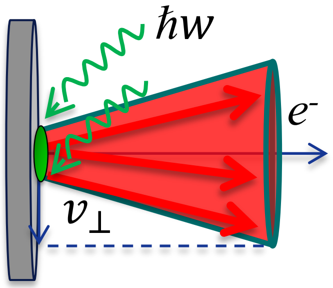


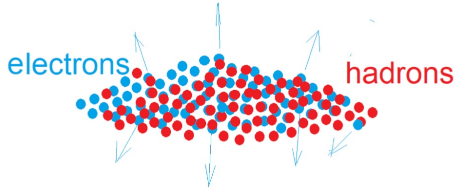


Electron-Ion Collider (EIC)
- nucleon spin structure
- parity-violating mechanisms

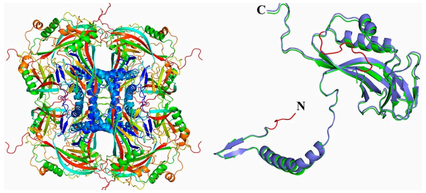
- prompt response time + low mean transverse energy (high-brightness applications)

$$MTE = \frac{m\langle v_\perp^2 \rangle}{2}$$

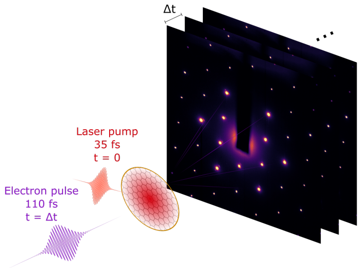




Electron cooling of hadron beams
reduction of emittance of hadron beams



X-ray Free Electron Laser (XFEL)
- protein crystallography
- cell biology



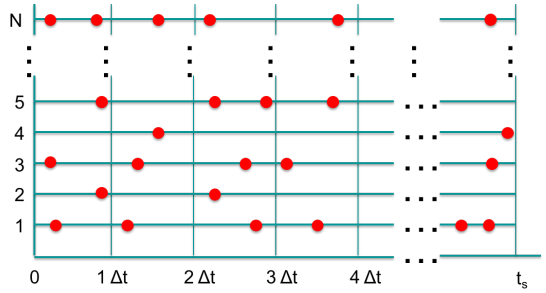
Ultrafast Electron Diffraction (UED)
dynamical changes of material structure

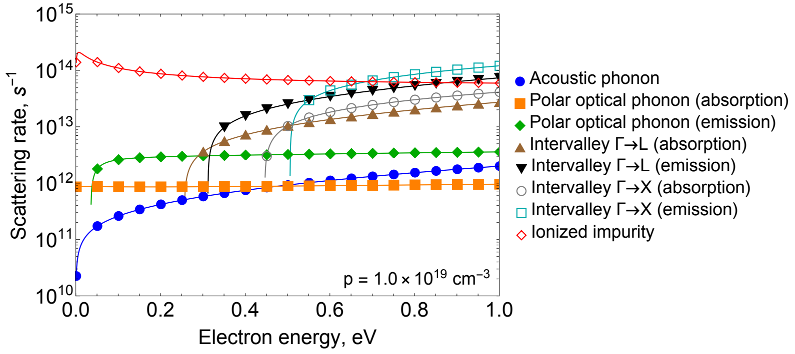
- robustness + long operational lifetime (5-100 MV/m to extract ~ 50-1000 pC/mm^2 of charge densities/bunch)

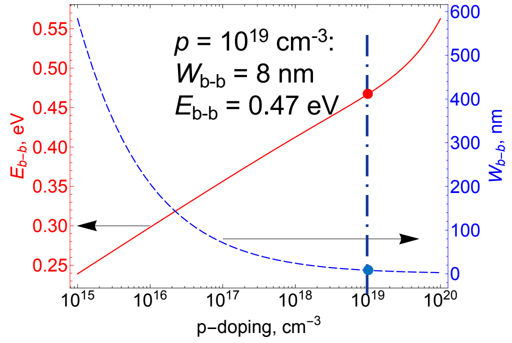
Monte Carlo approach for modeling photoemission from semiconductors

Photocathode Physics for Photoinjectors (P3) Workshop at SLAC November 11, 2021 chubenko@asu.edu

Transport

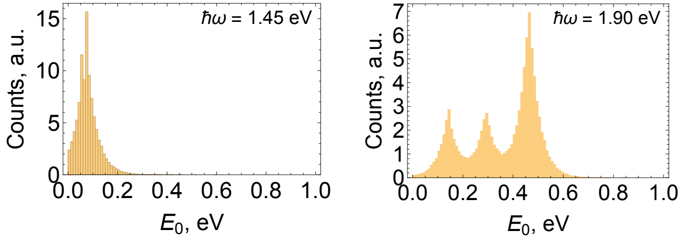




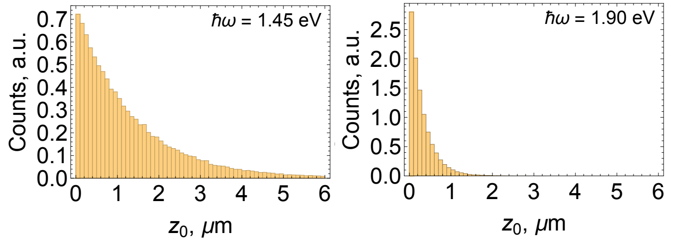


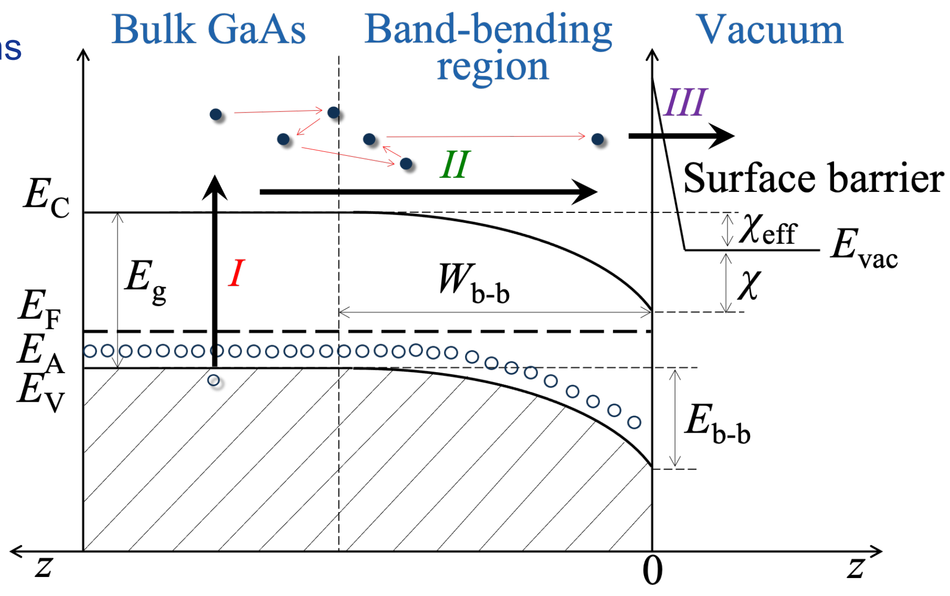
Photoexcitation

Initial energy distribution of photoexcited electrons

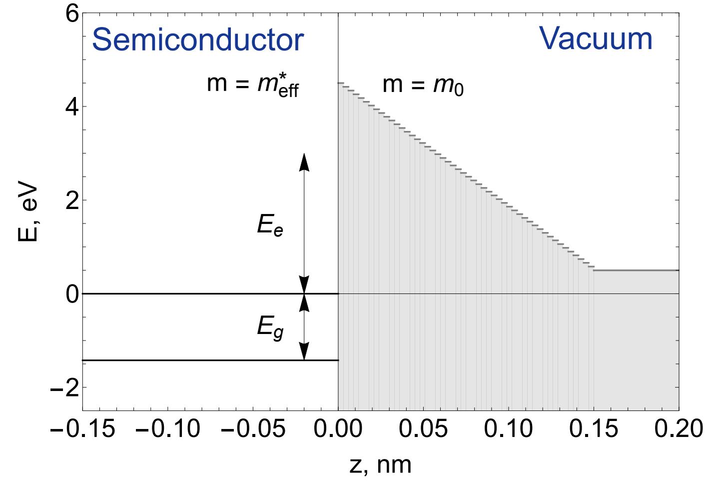


Initial electron distribution in real space





Emission



Photoemission from p-type NEA GaAs: I – photoexcitation, II – transport, III – emission.

Monte Carlo approach for modeling photoemission from semiconductors

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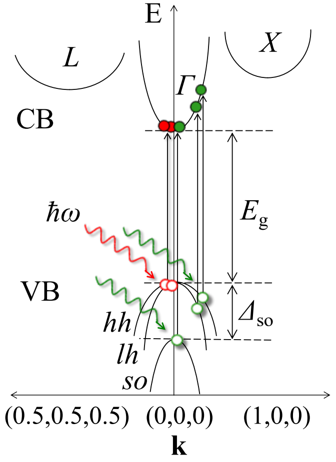
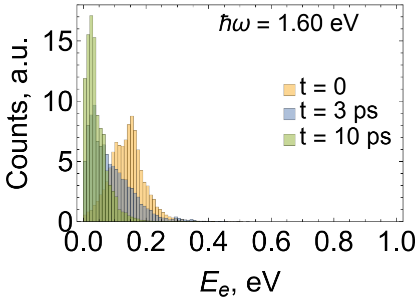
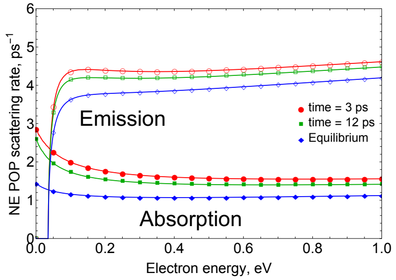
Advantages of Monte Carlo approach:

- QE, ESP, MTE, and response time can be simulated simultaneously as a function of $\hbar\omega$, N_a, χ, T.

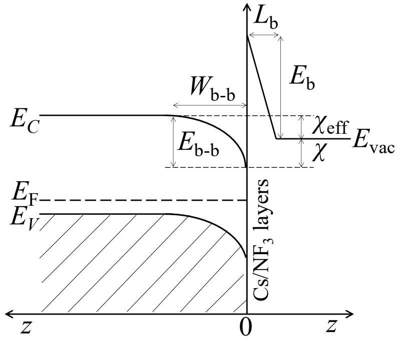


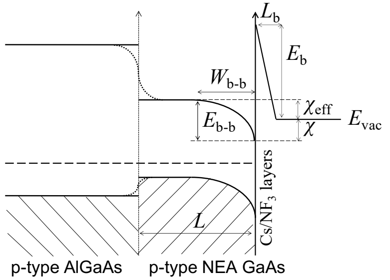
- Accounts for the subtleties of the material band structure.
- Does not require *a priori* assumption about the particle distribution functions.





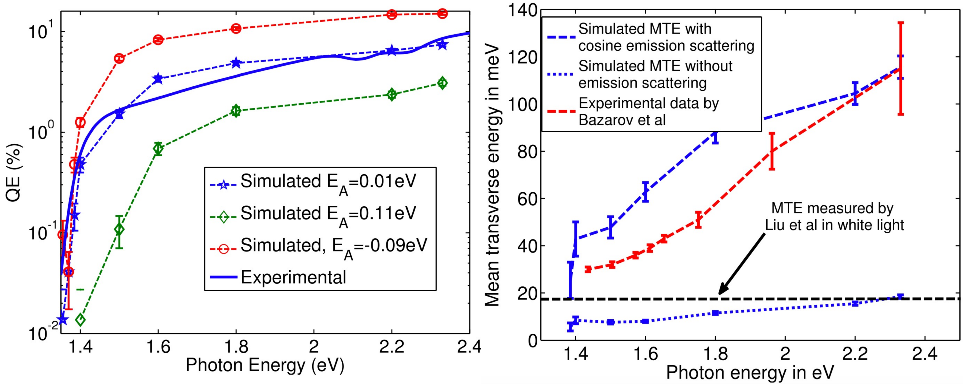
- Can be easily modified to include different scattering mechanisms to model both steady-state and non-equilibrium conditions.
- Accounts for the surface effects.
- Can be applied to both bulk and thin layers.



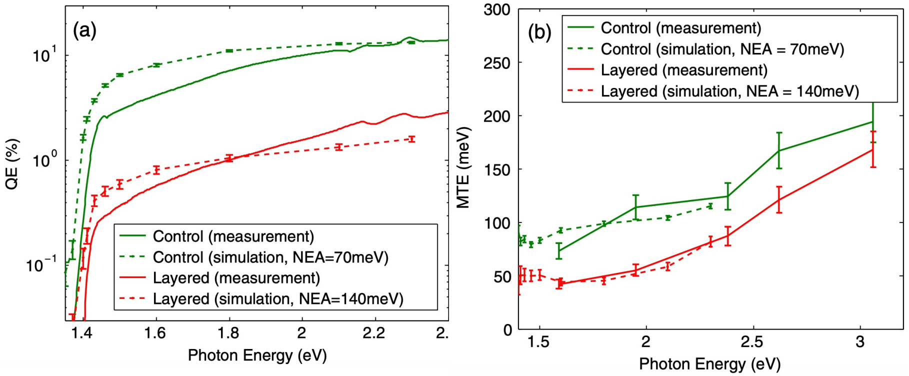


Monte Carlo approach for modeling photoemission from semiconductors

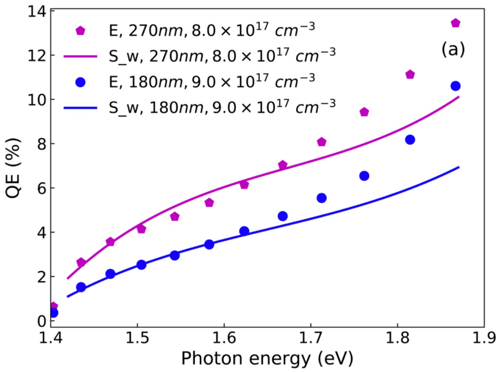
Provides good agreement with experimental data:



Karkare et al, J. Appl. Phys. **113**, 104904 (2013)

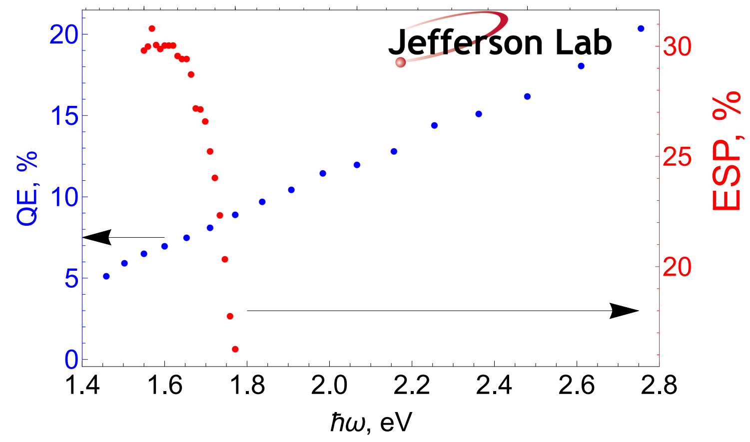


Karkare et al, Phys. Rev. Lett. **112**, 097601 (2014)



Liu & Wang, J. Appl. Phys. **126**, 075706 (2019)

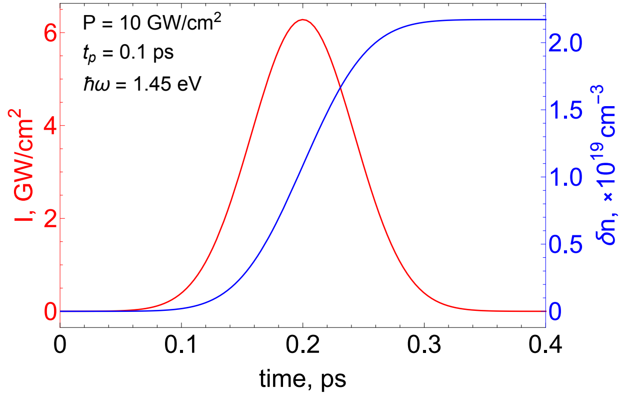
Application to spin-polarized photoemission?

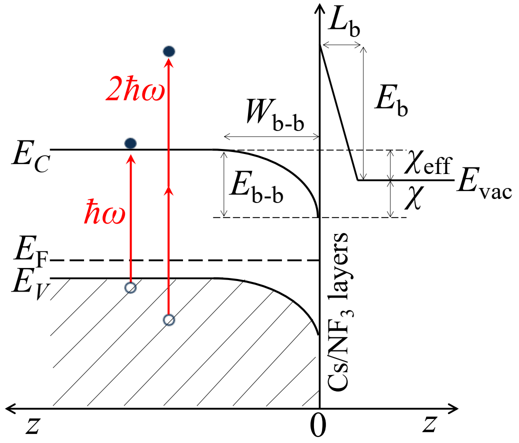


Characteristic behavior of experimental QE and ESP from NEA GaAs.

Application to non-linear photoemission?

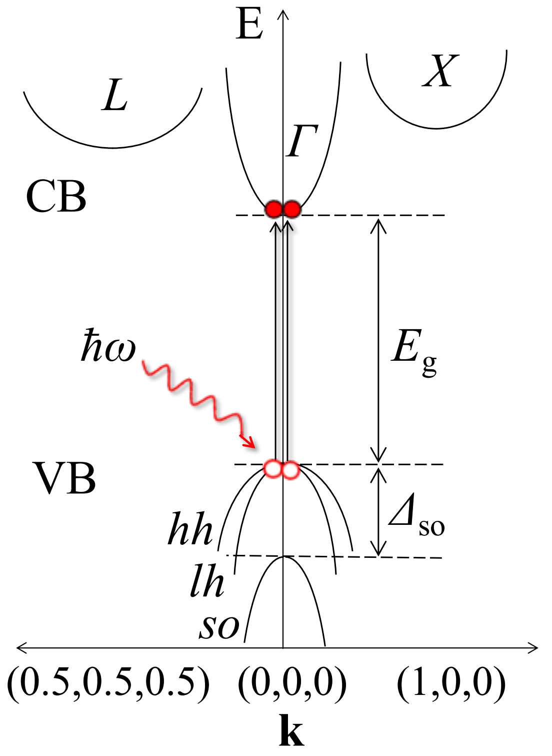
Ultra-short-pulse laser of high fluence

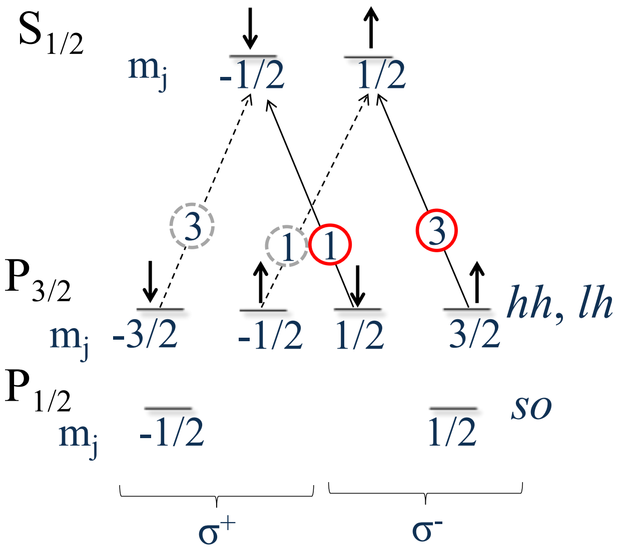




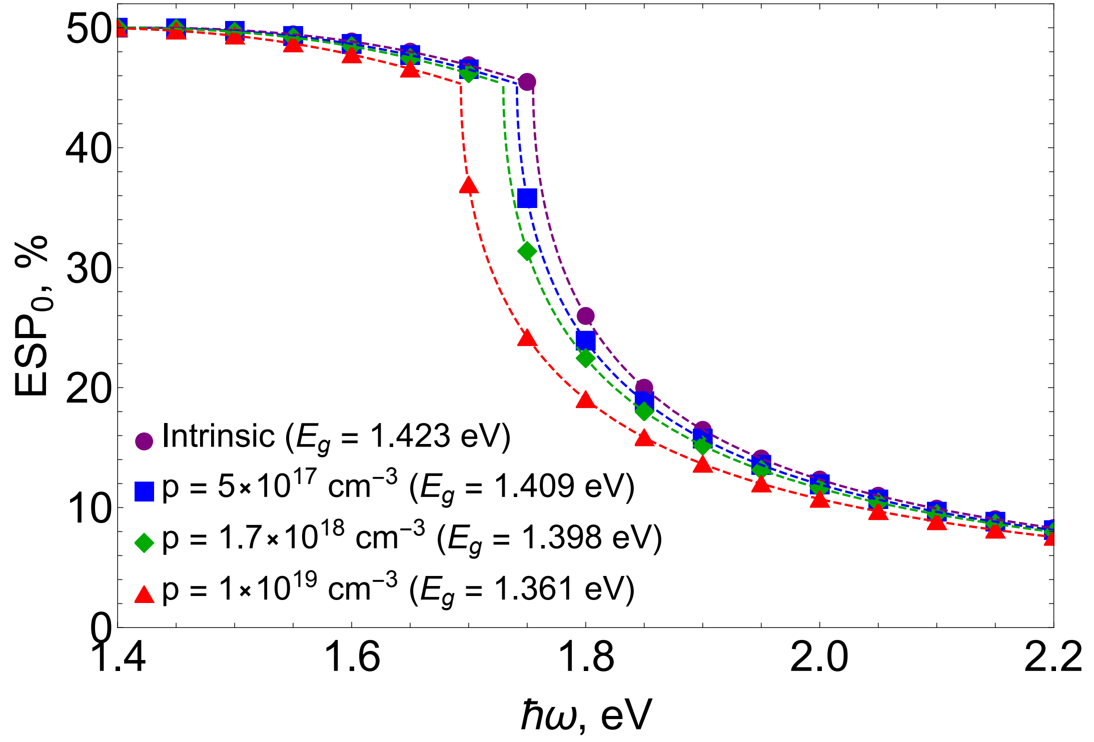
Monte Carlo study of spin-polarized photoemission from GaAs

Initial electron spin polarization ESP_0:





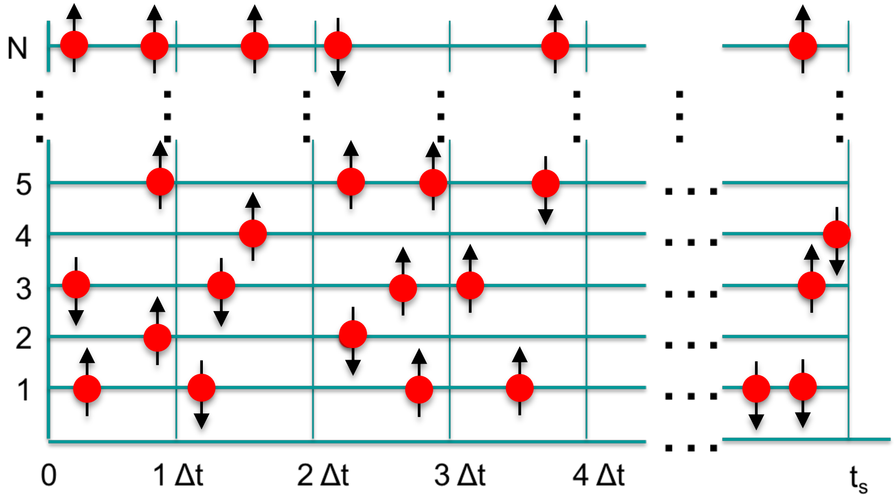
$$\hbar\omega \approx E_g \;\rightarrow\; ESP_0 = \left|\frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}\right| = \left|\frac{3-1}{3+1}\right| = 50\%$$

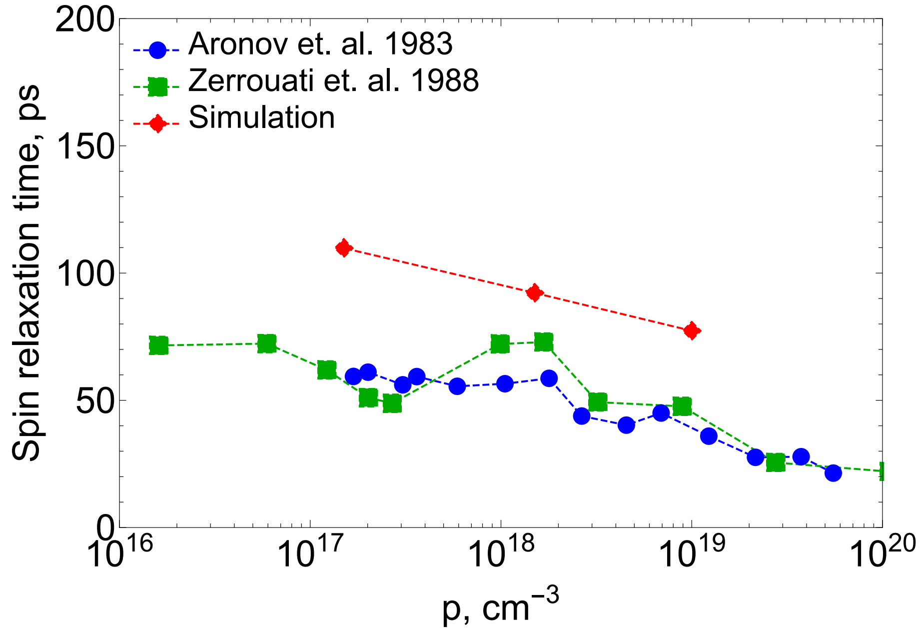


Chubenko et al. J. Appl. Phys. **130**, 063101 (2021)
D'yakonov and Perel', Sov. Phys. JETP **33**, 1053 (1971)

Spin relaxation mechanisms:

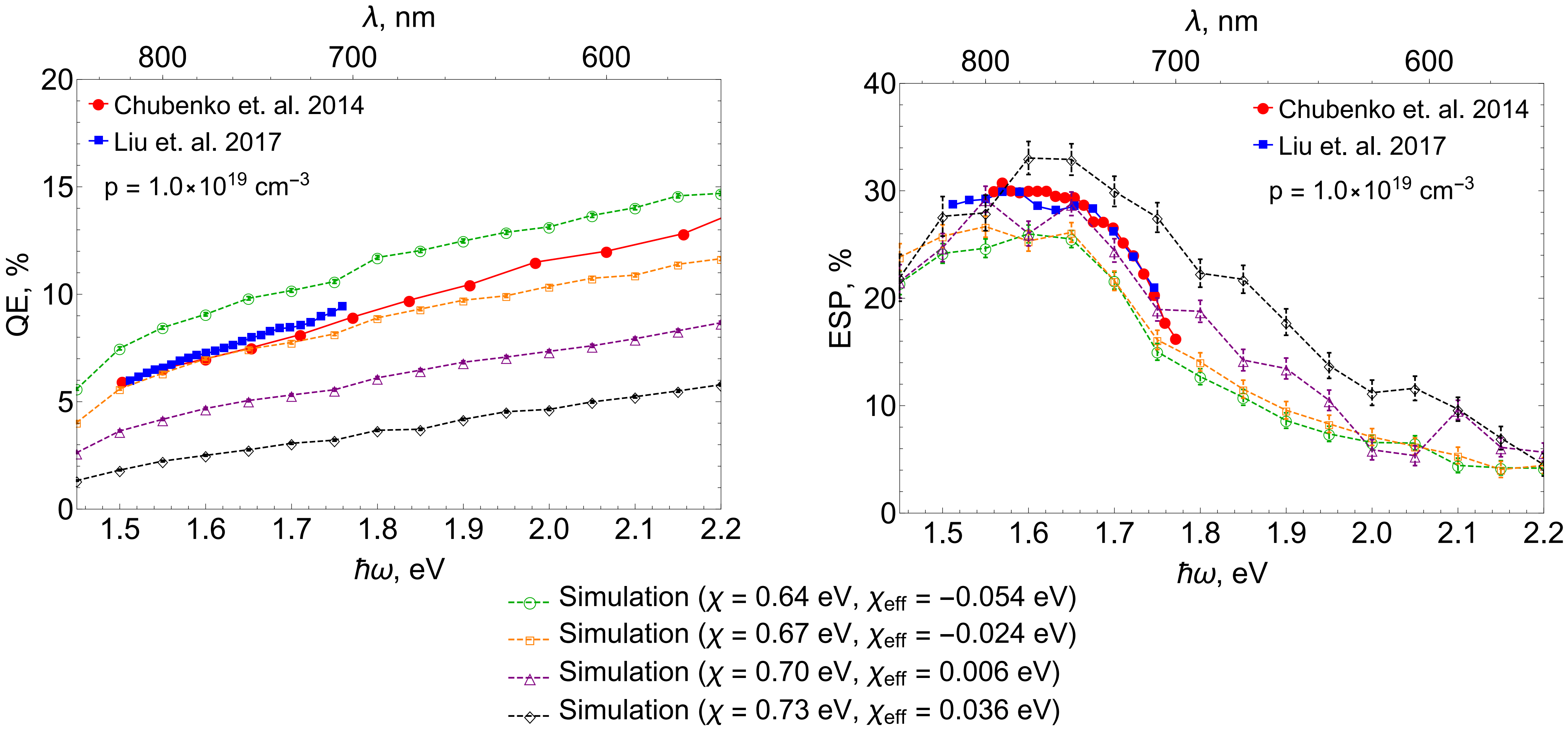
- Elliott-Yafet (EY): takes into account the mixing of wave functions with different spins as a result of spin-orbit interaction.
- D'yakonov-Perel (DP): arises due to the lack of an inversion center in some semiconductors which leads to splitting of the spin states of the CB at k ≠ 0.
- Bir-Aronov-Pikus (BIP): originates from the exchange interaction of electrons with holes.





Chubenko et al. J. Appl. Phys. **130**, 063101 (2021)

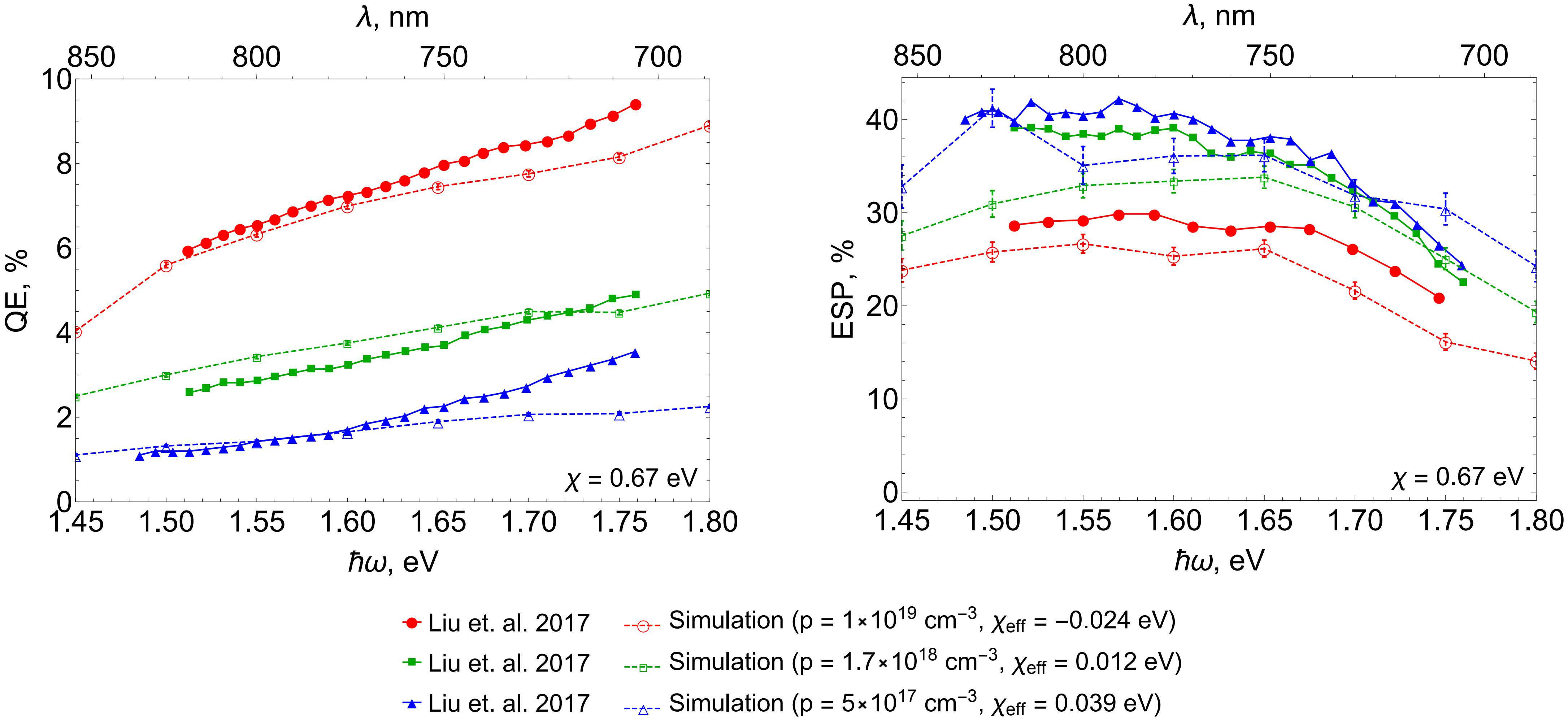
Comparison with experiment: QE and ESP from p-type GaAs for different electron affinity levels



Chubenko et al. J. Appl. Phys. **130**, 063101 (2021)

Monte Carlo study of spin-polarized photoemission from GaAs

Comparison with experiment: QE and ESP from p-type GaAs for different doping densities



Future applications of spin-polarized Monte Carlo model

High-QE, high-ESP from GaAs-based SuperLattice structures activated to NEA:

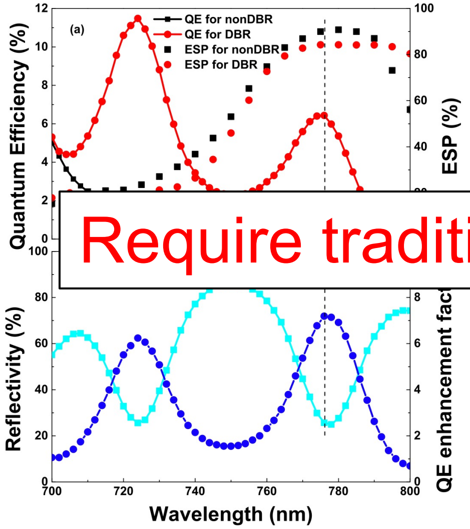


TABLE I. Figure of merit for polarized electron sources.

Cathode	Reference	P (%)	QE (%)	P^2QE (%)
$Al_{0.19}In_{0.2}GaAs-Al_{0.4}GaAs$	St. Peterburg	92	0.85	0.72
$GaAs-gaAsP_{0.35}$ (with DBR)	JLab/SVT	84	6.4	4.52

Require traditional Cs-based activation to NEA!

Liu et al. Appl. Phys. Lett. **109**, 252104 (2016)

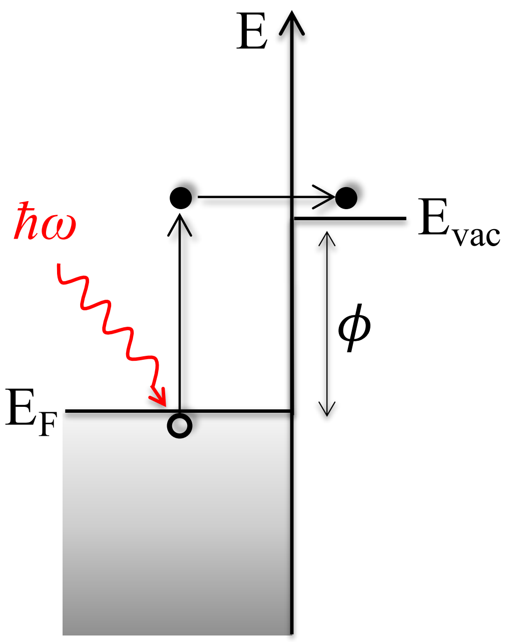
Monte Carlo investigation of novel spin-polarized electron sources:

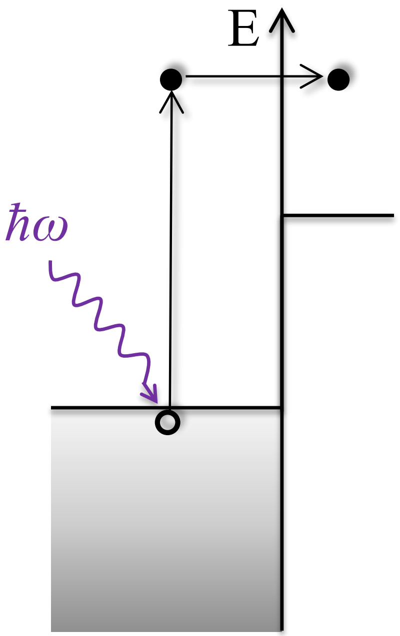
- ✓ Effective/fast modeling of spin-polarized photoemission: C + MPI to run in parallel at HPC cluster.
- ✓ Good agreement with available experimental data → creates a paradigm for future studies:
  - predict spin-polarized photoemission from other known spin-polarized materials and/or structures, which do not require traditional surface preparation (Luca Cultrera’s talk, Session C).
  - Monte Carlo + *ab initio* calculations to enable effective exploration of other potential materials to produce spin-polarized electrons.

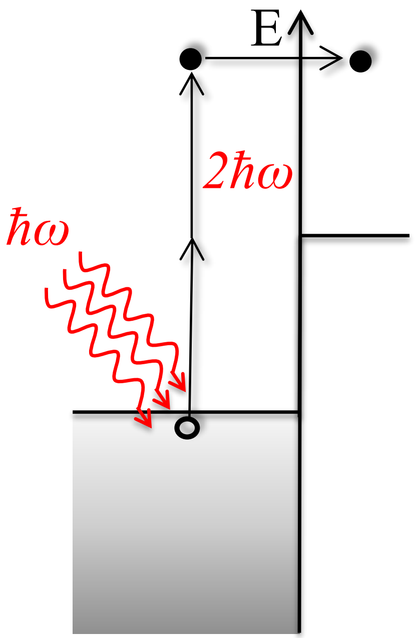
Monte Carlo study of non-linear photoemission from semiconductor photocathodes

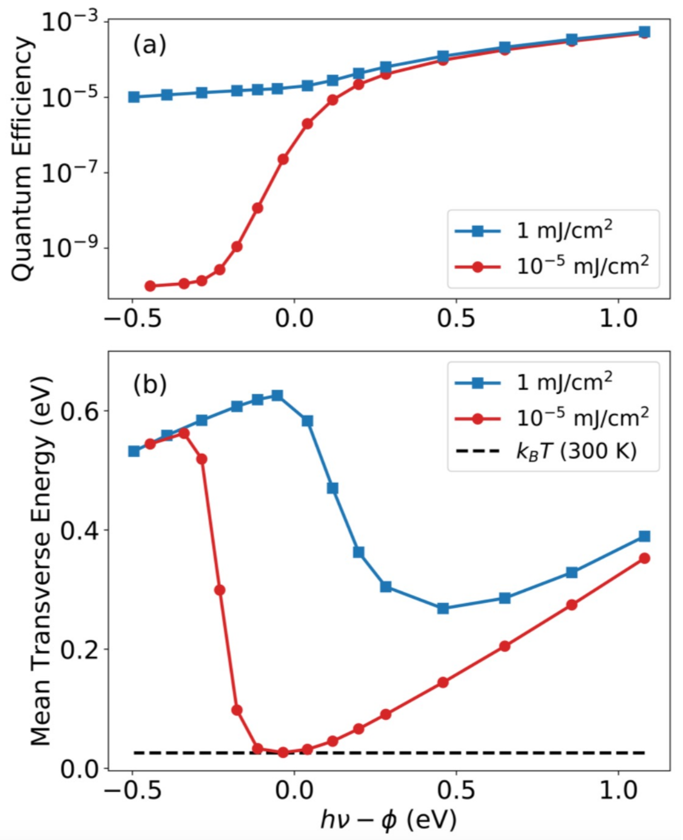
Non-linear effects is metals

Metals:









$\hbar\omega \approx \phi \quad \Rightarrow$ MTE $\approx k_B T$

Low MTE, but low QE

$\hbar\omega \gg \phi \quad \Rightarrow$ MTE $\approx (\hbar\omega - \phi)/3$

High QE, but high MTE

sub-ps pulse, 1 mJ/cm^2

Non-monotonic MTE

Bae et al. J. App. Phys. **124**, 244903 (2018)

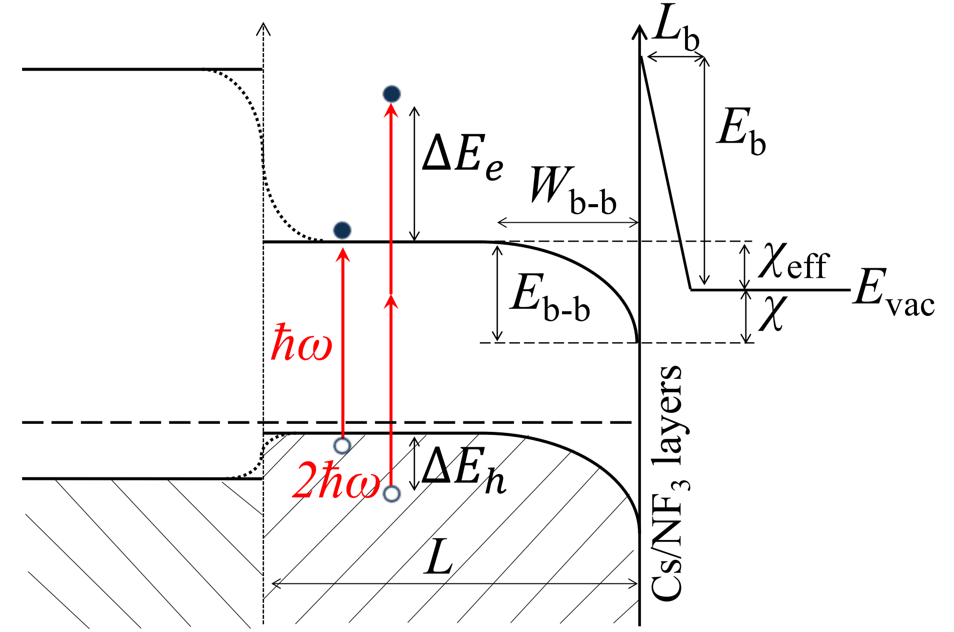
Monte Carlo study of laser-induced heating effects in semiconductor photocathodes

Semiconductors:

Ultra-short-pulse laser of high fluence:

1. High density of electron-hole pairs
   - Carrier-carrier (C-C) interactions
   - Non-equilibrium polar optical phonons (NE POPs)
   - Degeneracy effects
   - Screening effects
   - Auger recombination
2. High excess energy
   - Additional source of kinetic energy leading to carrier heating

$QE_{PEA} \approx 0.01\%$ ⇨ $N_\gamma \approx 10^{16}$ cm^{-2} in a 1-ps pulse
(P ≈ 2.4 GW/cm^2)
$N_{ex} \approx 10^{18}$ -10^{20} cm^{-3}



$$\Delta E = \hbar\omega - E_g = \Delta E_e + \Delta E_h$$
$$\Delta E = 2\hbar\omega - E_g = \Delta E_e + \Delta E_h$$

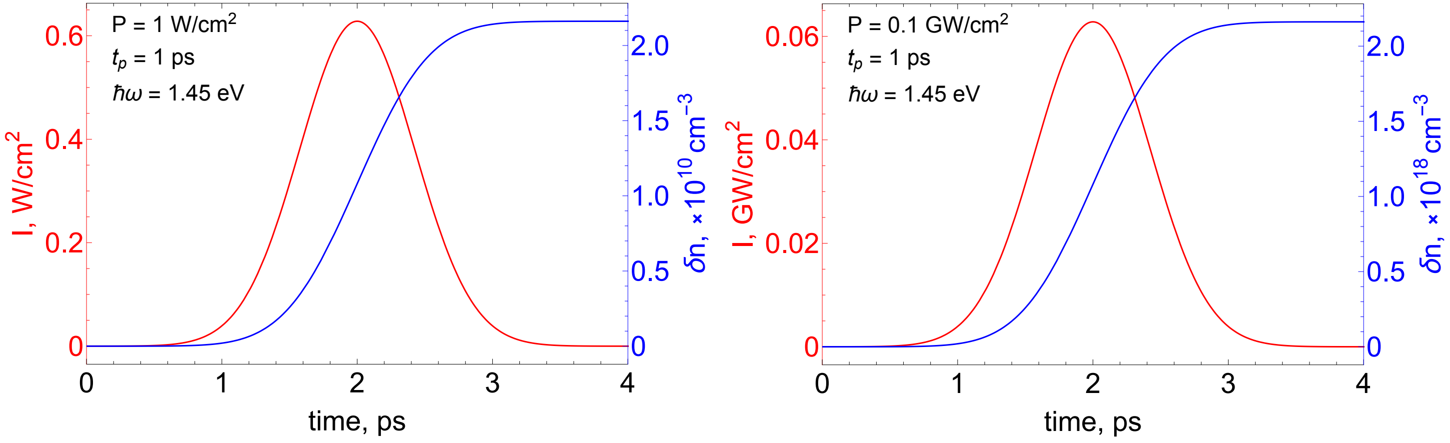
Detailed modeling is required to provide quantitative estimation of the mechanisms limiting beam brightness of semiconductor photocathodes under high laser fluences.

M. A. Osman and D. K. Ferry, Phys. Rev. B36, 6018 (1987).
P. Lugli and D. K. Ferry, Physica117B&118B, 251 (1983).
R. Brunetti, C. Jacoboni, A. Matulionis, and V. Dienys, Physica134B, 369 (1985).
R. P. Joshi, R. O. Grondin, and D. K. Ferry, Phys. Rev. B42,5685 (1990).

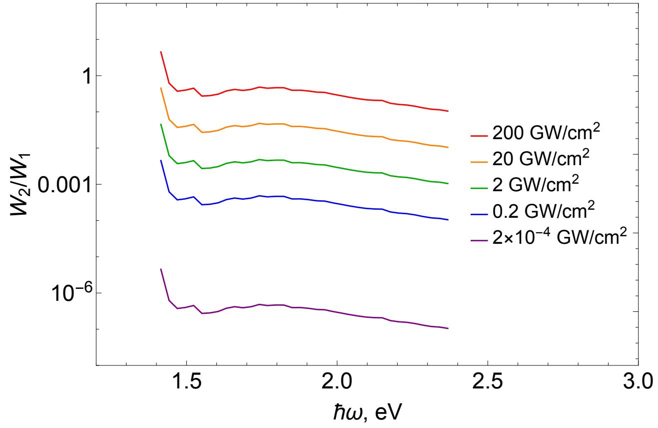
Monte Carlo study of laser-induced heating effects in semiconductor photocathodes

Photoexcitation:

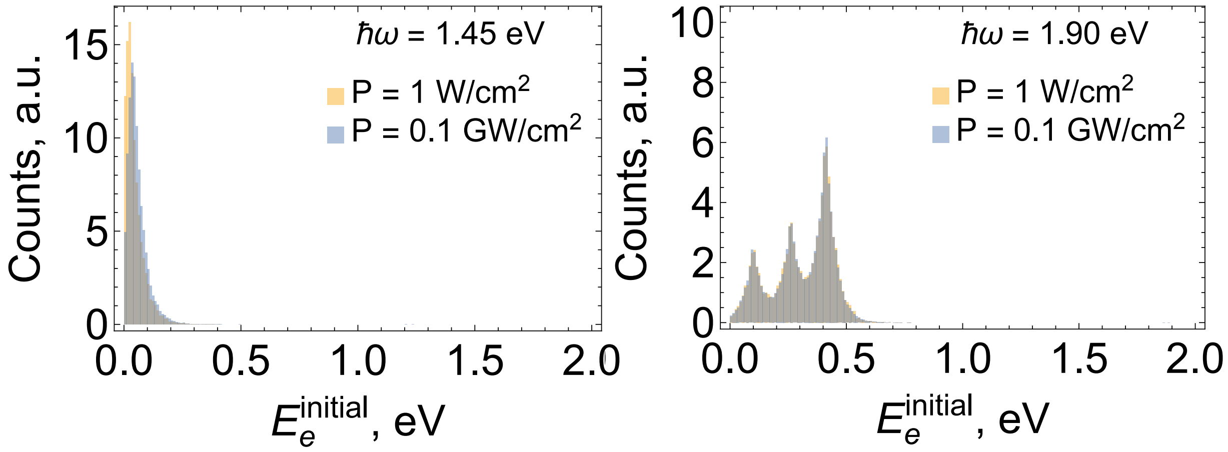
Gaussian laser pulse of different power density *P*



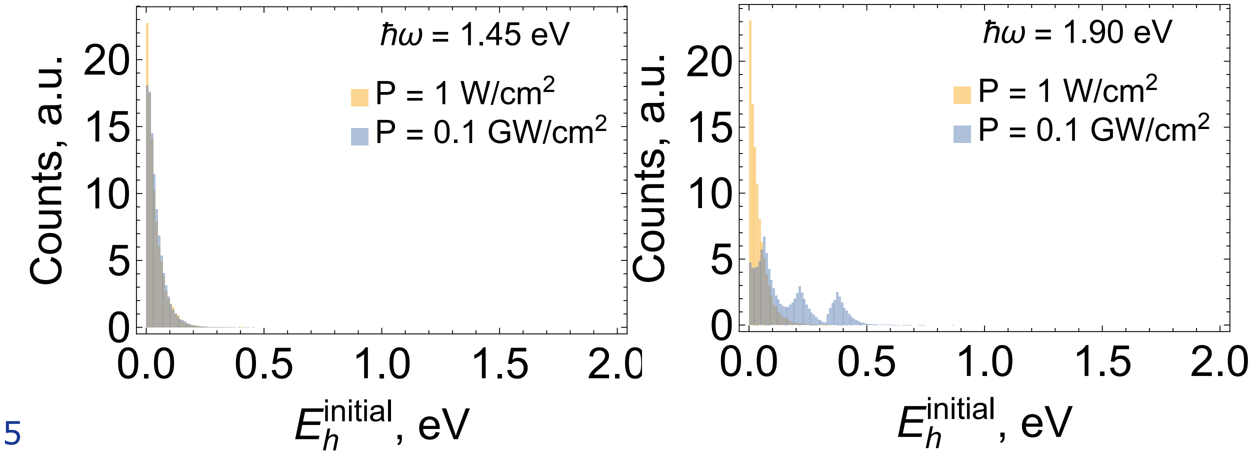
Ratio of two-photon transition rate W_2 to the one-photon transition rate W_1 for various laser power densities inside GaAs (*ab initio* calc. by J. Kevin Nangoi).



Initial energy distribution of electrons



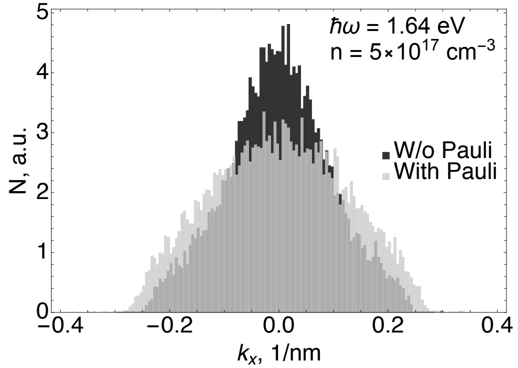
Initial energy distribution of holes in p-doped GaAs ($N_a = 10^{18}$ cm^{-3})



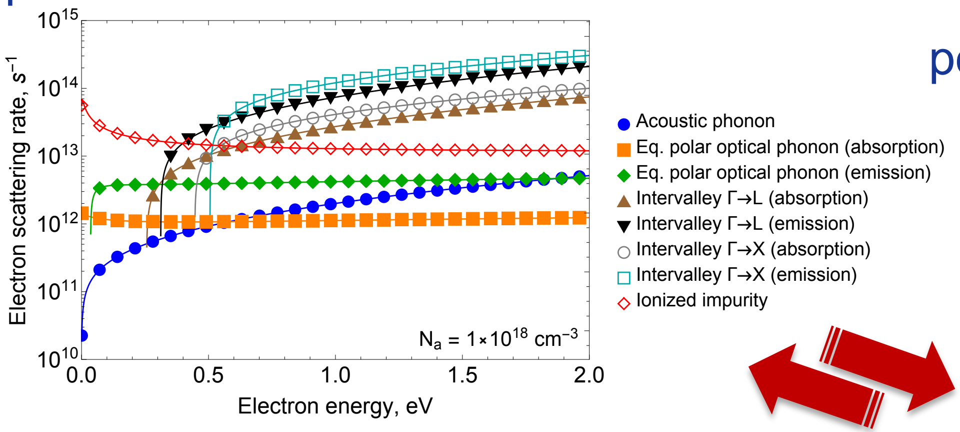
Monte Carlo study of laser-induced heating effects in semiconductor photocathodes

Transport:

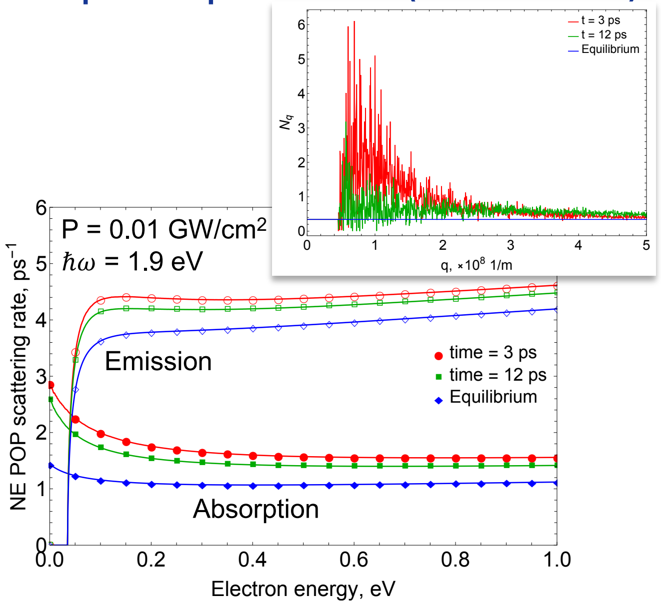
Pauli exclusion principle



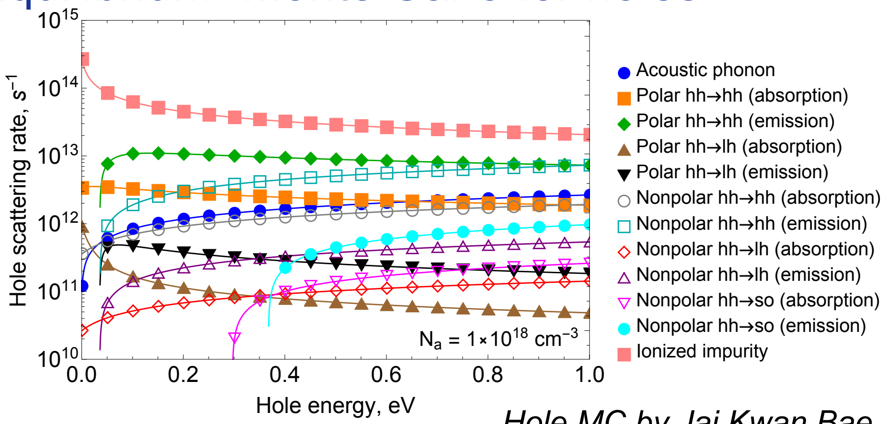
"Equilibrium" Monte Carlo for electrons



Non-equilibrium polar optical phonons (NE POPs)



"Equilibrium" Monte Carlo for holes



Hole MC by Jai Kwan Bae

Monte Carlo study of laser-induced heating effects in semiconductor photocathodes

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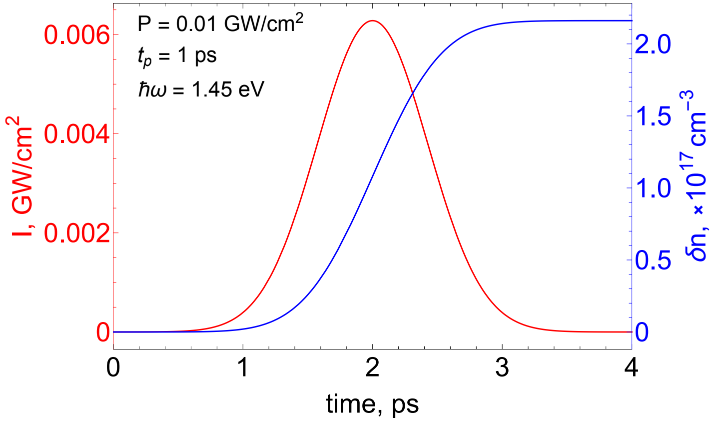
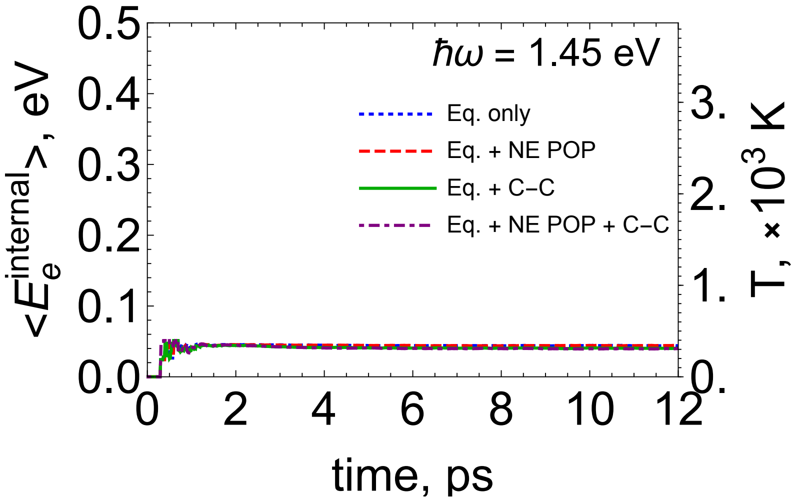
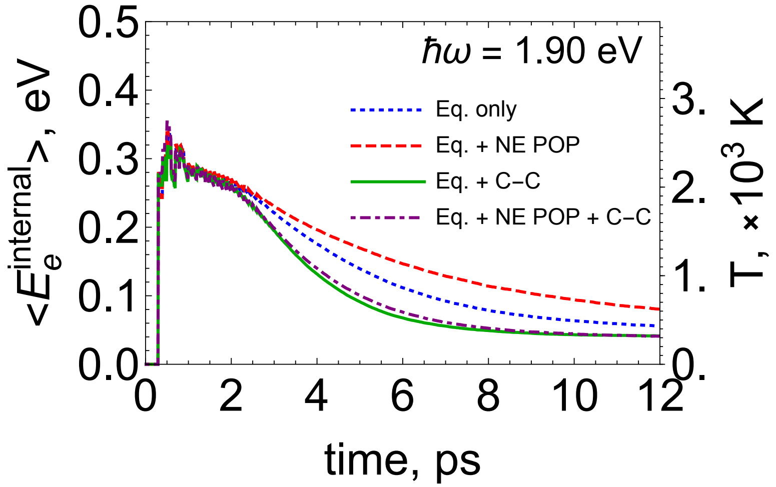
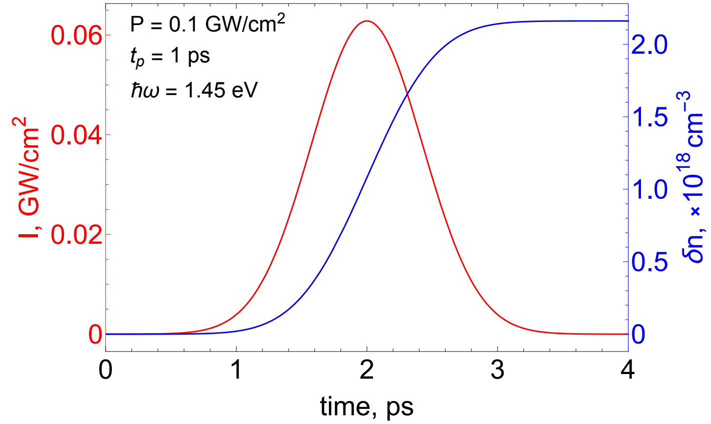
Preliminary results:

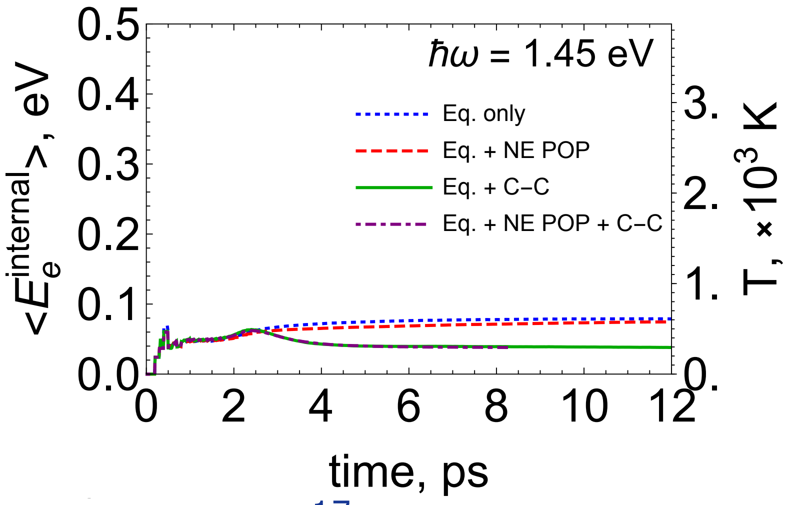
$$\langle E_e^{\text{internal}} \rangle = \frac{3}{2} k_B T$$

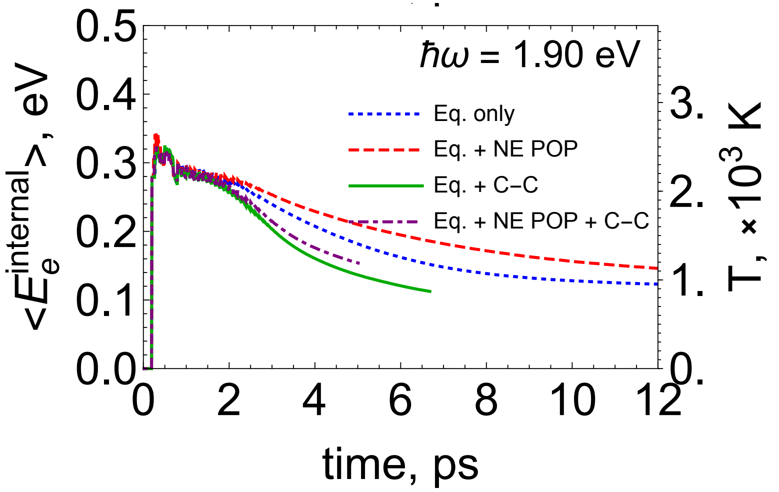




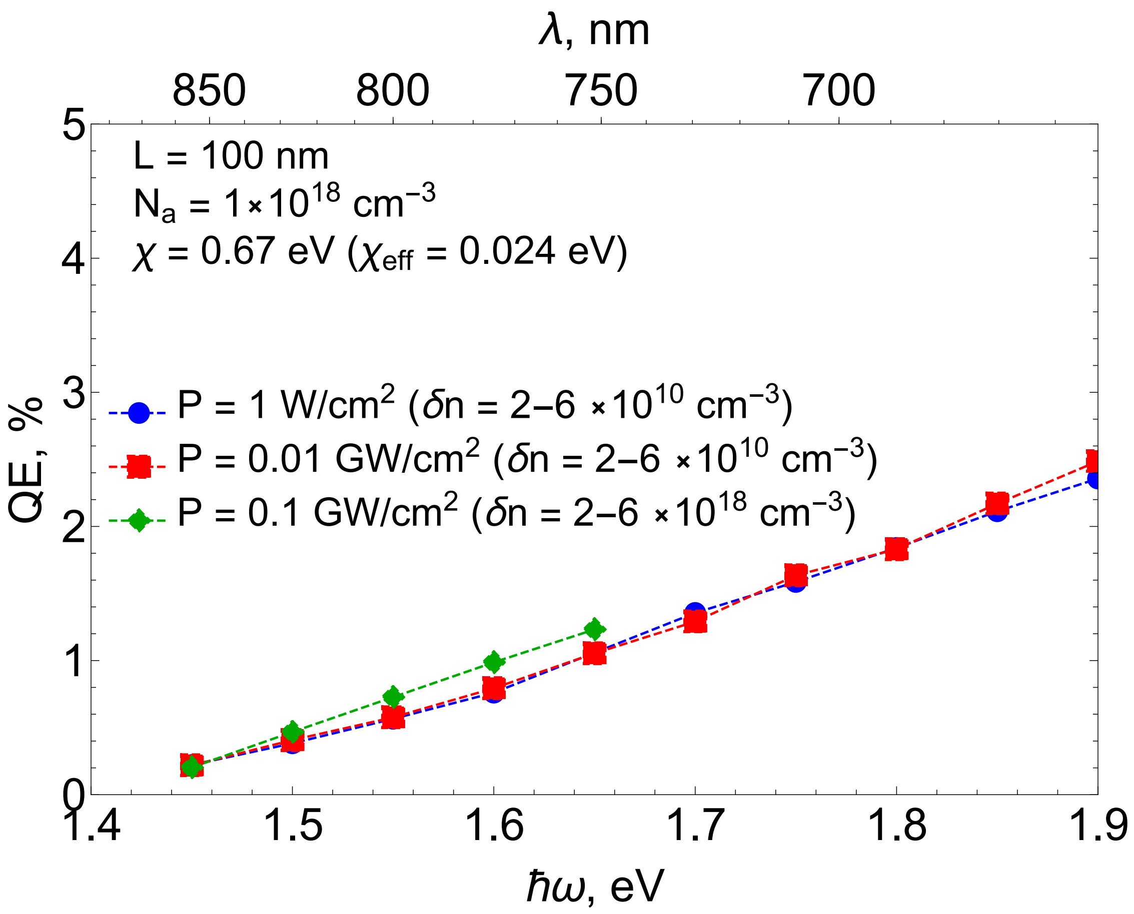


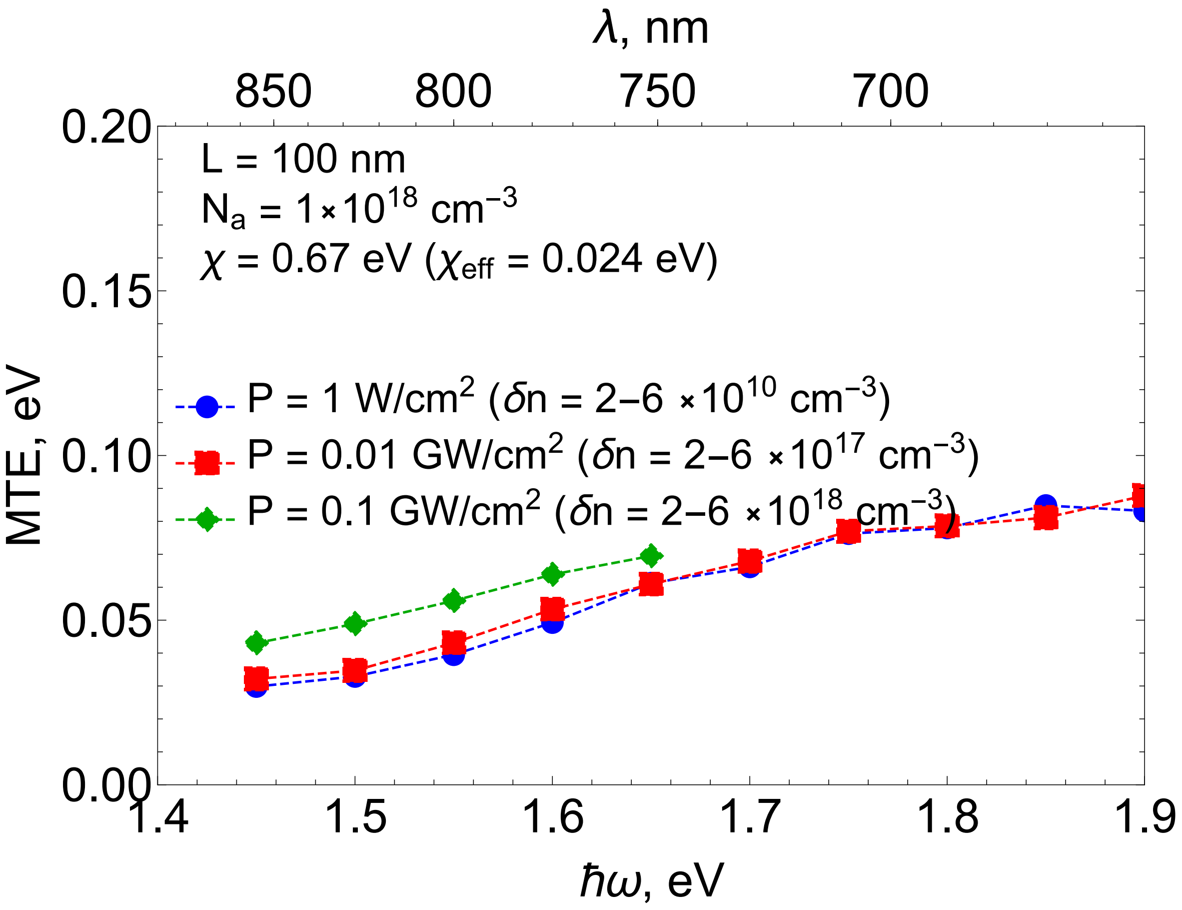






Preliminary results:



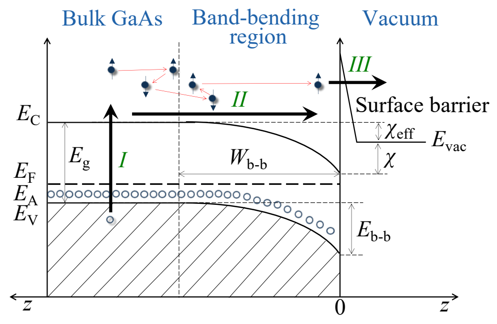


Low-electron-affinity semiconductor photocathodes are better candidates to operate under high laser fluences.*

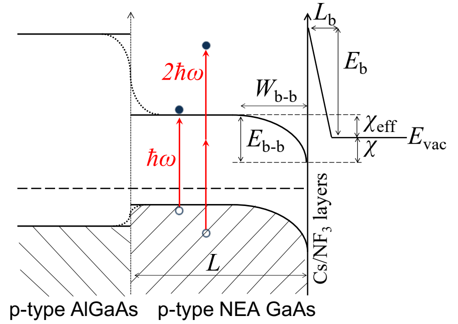
*Preliminary

Summary and future directions

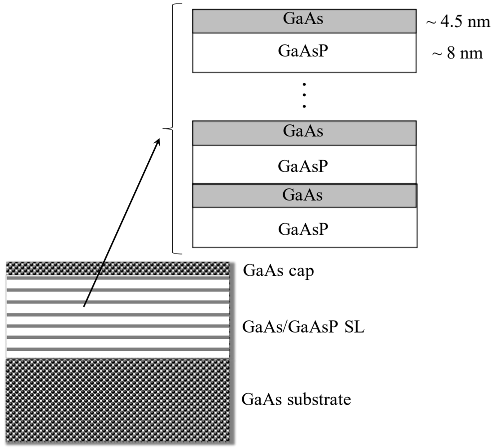
- The detailed Monte Carlo model of photoemission has been developed to model main electron emission characteristics of semiconductor photocathodes. The model provides good agreement with experimental data for bulk NEA GaAs.



- The work in progress to study effects of non-linear photoemission on QE and MTE of thin GaAs structures for high-current high-brightness applications. The model can be modified further to study non-linear effects in other bright photocathodes like alkali antimonide semiconductors.



- The developed Monte Carlo model is the semi-classical approach, which is applicable when the applied and/or built-in potentials vary slowly on the scale of electron's wavelength (~ 29 nm in GaAs), otherwise the wave phenomena such as reflections and tunneling are present and carriers must be treated quantum mechanically. Therefore, the full quantum methods like Non-equilibrium Green's Function Technique or Wigner Monte Carlo can be employed to enable modeling of nanostructured photocathodes.



Acknowledgements

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