Northern Illinois University

Monte Carlo Modeling of Spin-Polarized Photoemission

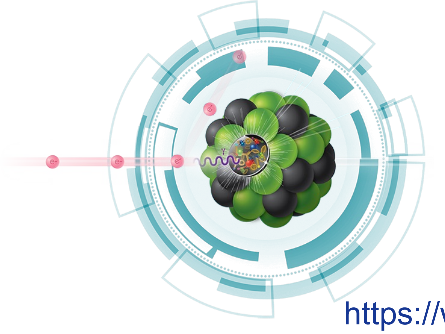
Oksana Chubenko

Department of Physics, Northern Illinois University, DeKalb, IL 60115

Spin-polarized electron beams and their applications

Particle Physics

- probe the structure of subatomic particles
- study fundamental forces
- explore the properties of matter



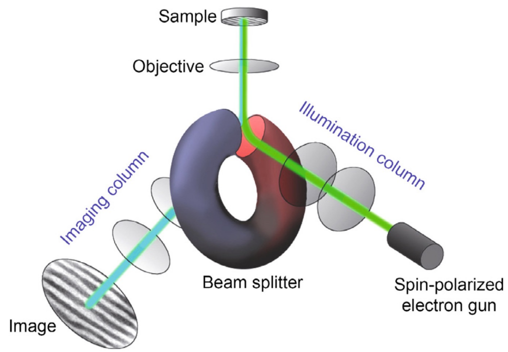
https://www.bnl.gov/eic/

Spin-Polarized Scanning Tunneling Microscopy (SP-STM)

- study the magnetic properties and electronic structure of nanostructures at the atomic and molecular level

Spin-Polarized Low-Energy Electron Microscopy (SP-LEEM)

- imaging magnetic microstructures at surfaces and in thin films.



Rougemaille and Schmid, Eur. Phys. J. Appl. Phys. 50, 20101 (2010)

Ultrafast Spin-Polarized Low-Energy Electron Diffraction (LEED)

- enable us to understand the correlation between structure and magnetism in ultrafast processes on surfaces at the nanoscale

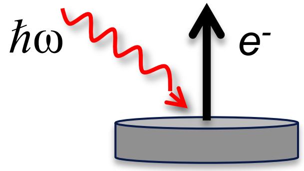
Materials Sciences

- investigate the electronic and magnetic properties of materials

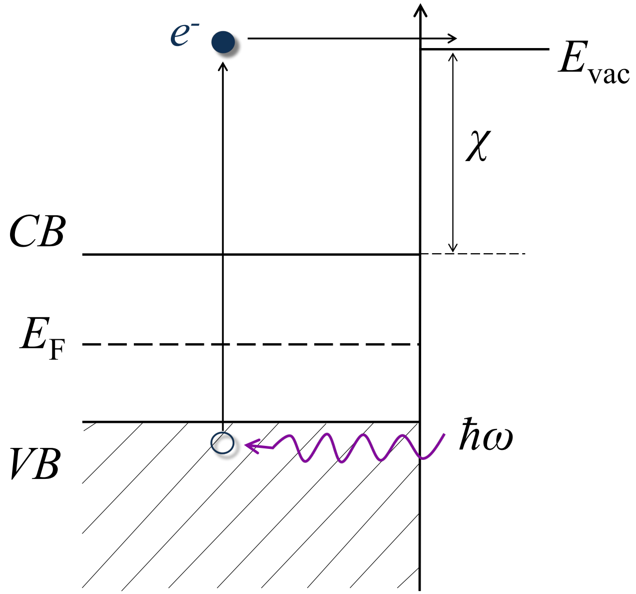
Requirements for efficient spin-polarized electron sources

- ***High Quantum Efficiency (QE)***

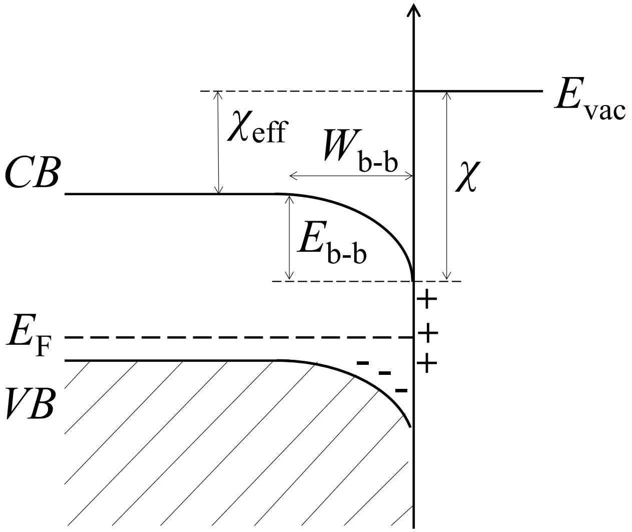
$$QE = \frac{N_{e^-}}{N_{\hbar\omega}}$$



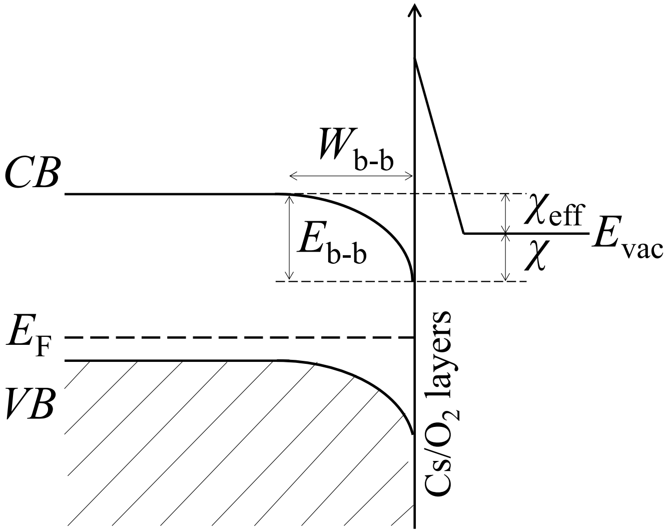
Intrinsic GaAs:



p-doped GaAs:



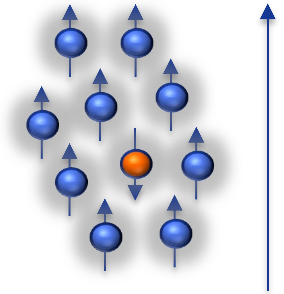
p-doped GaAs activated to NEA:



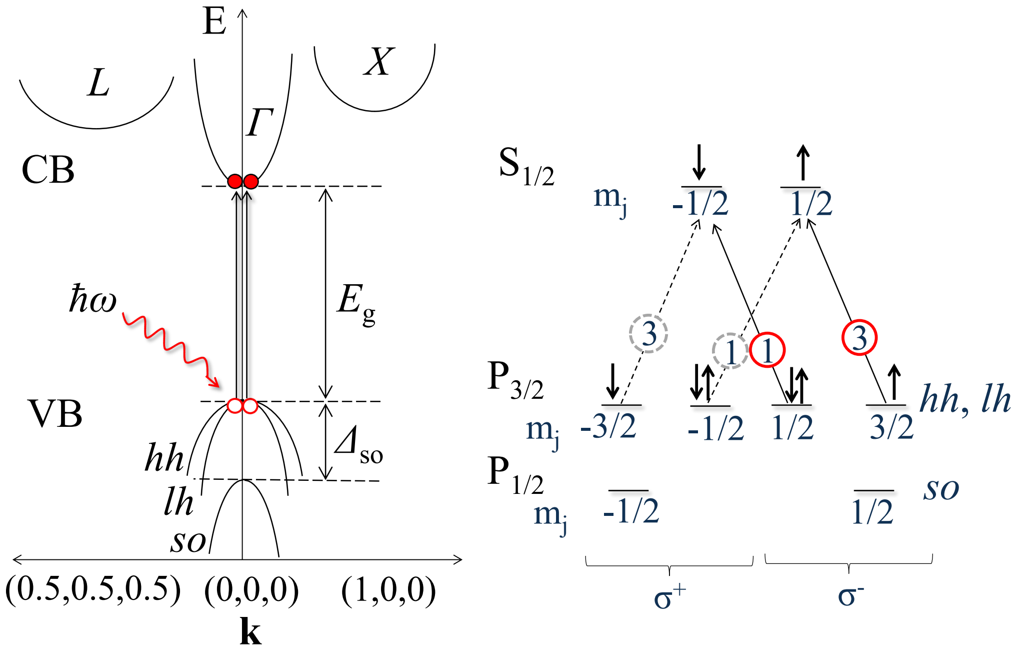
Requirements for efficient spin-polarized electron sources

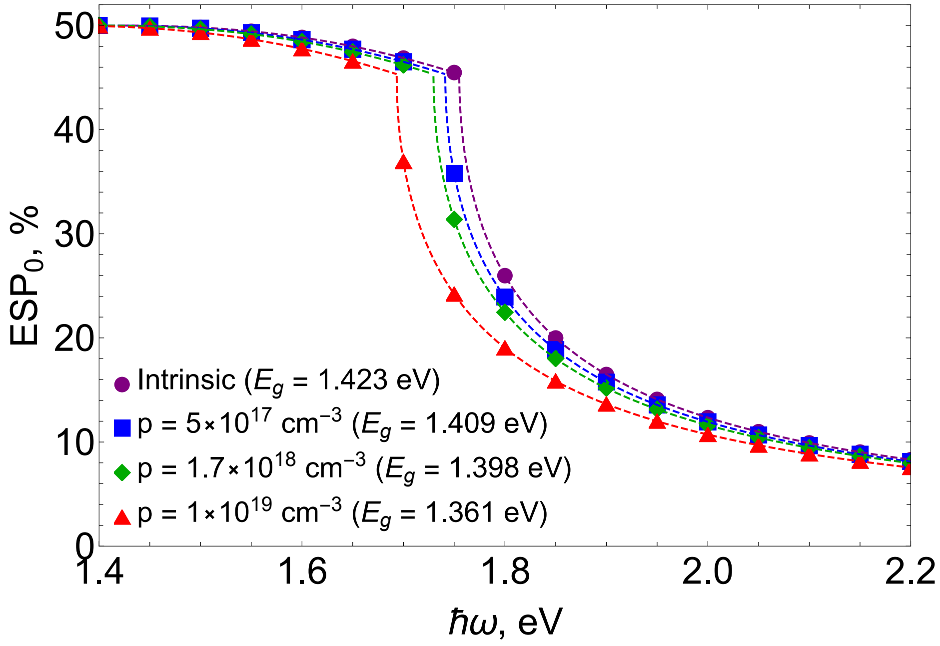
- ***High Electron Spin Polarization (ESP)***

$$ESP_0 = \left|\frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}\right|$$



Unstrained GaAs:





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

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

Requirements for efficient spin-polarized electron sources

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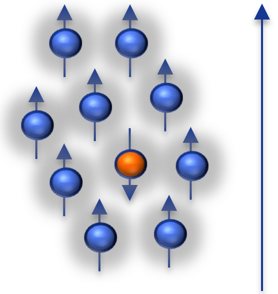
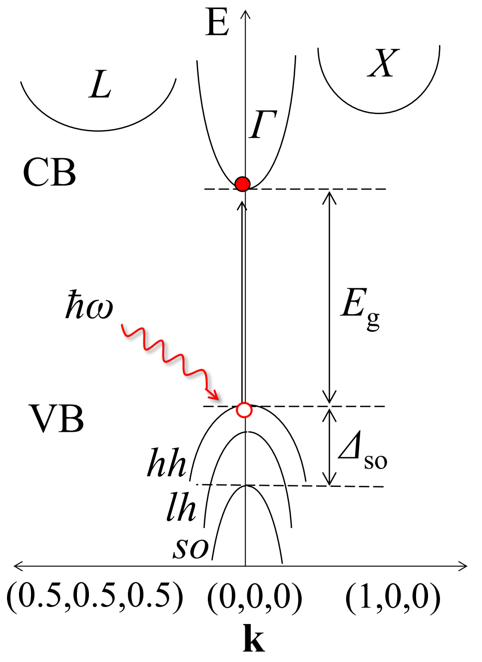
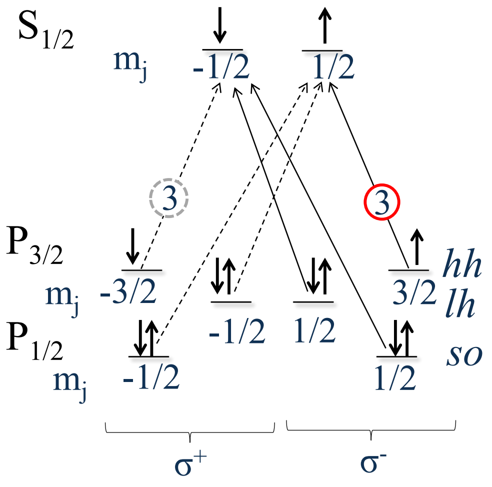
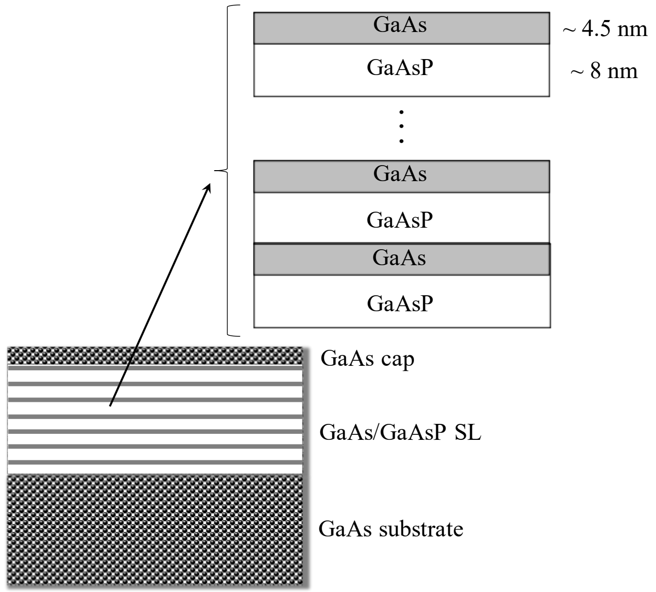


Strained GaAs:





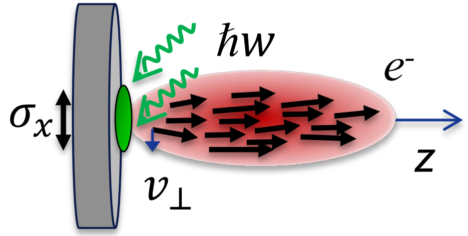


$$\hbar\omega \approx E_g \;\rightarrow\; ESP_0 = \left|\frac{3-0}{3-0}\right| = 100\%$$

Requirements for efficient spin-polarized electron sources

- ***High Brightness = high current + low Mean Transverse Energy (MTE)***

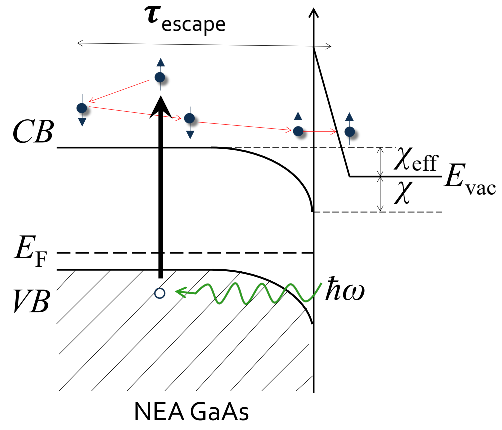
$$B_{5D,max} \propto \frac{I}{\epsilon_x \epsilon_y} \propto \frac{I}{\sigma_x \sigma_y MTE} \qquad MTE = \frac{m\langle v_\perp^2 \rangle}{2}$$



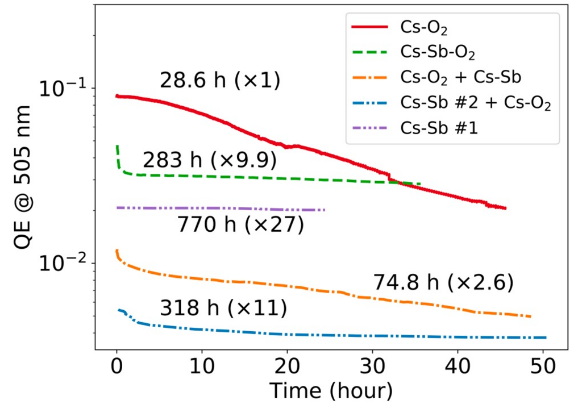
$$\epsilon_{x,y} = \sigma_{x,y}\sqrt{MTE/m_e c^2}$$

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

- ***Prompt response time***



- ***Robustness + long operational lifetime***



Bae et al. J. Appl. Phys. 127, 124901 (2020).

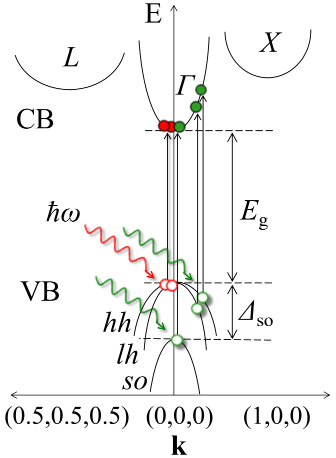
- ***Accessibility***

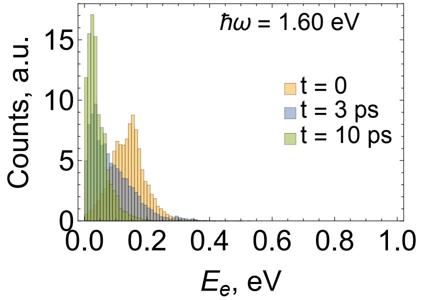
Monte Carlo approach for modeling spin-polarized photoemission from semiconductors

Advantages of Monte Carlo approach:

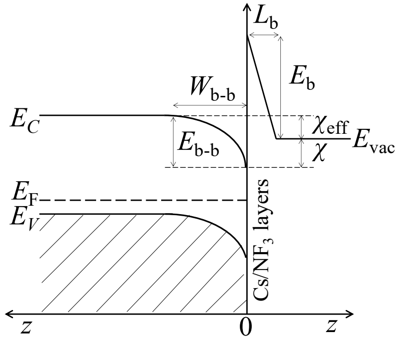
- QE, ESP, MTE, response time = *f*($\hbar\omega, p, \chi, T$).

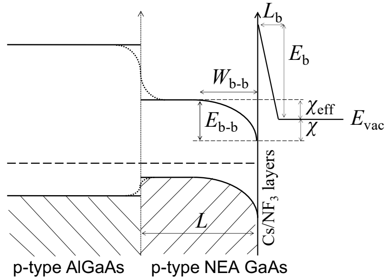
- Accounts for the subtleties of the material band structure.





- 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 spin-polarized photoemission from semiconductors

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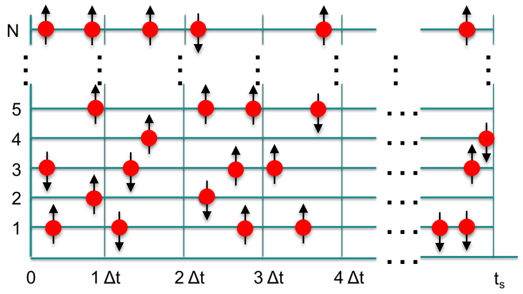
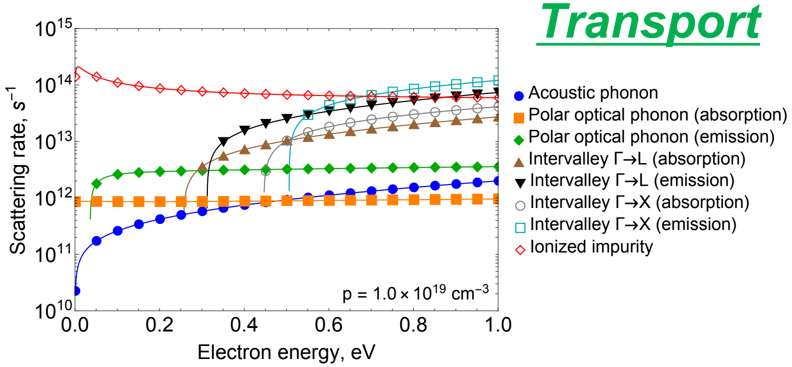
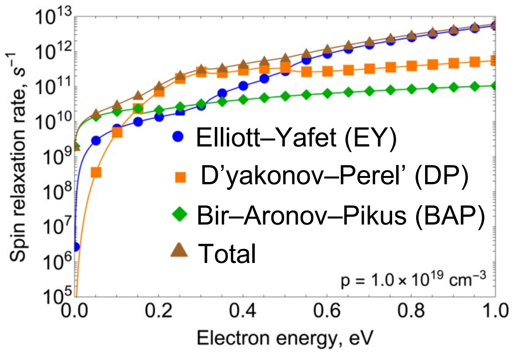
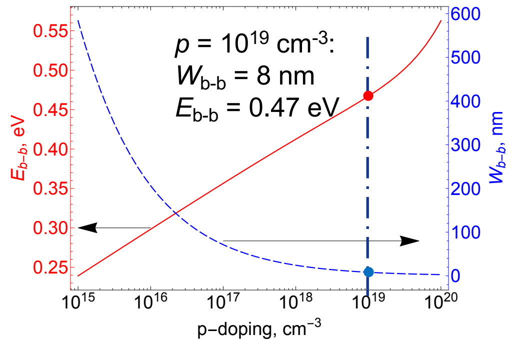




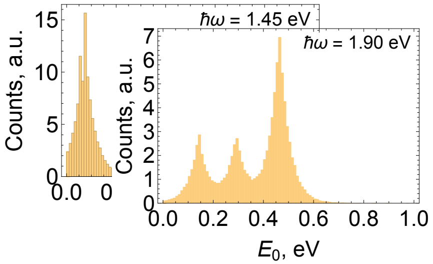
Transport



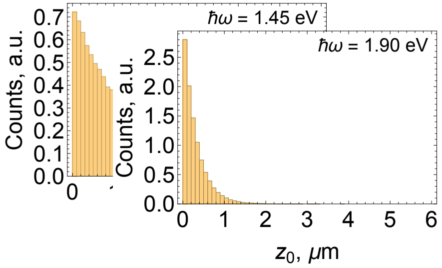


Photoexcitation

Initial energy distribution of photoexcited electrons

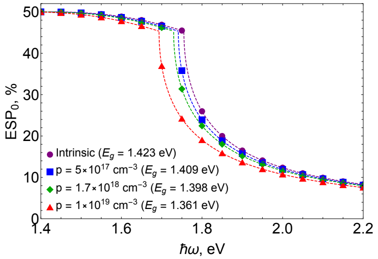


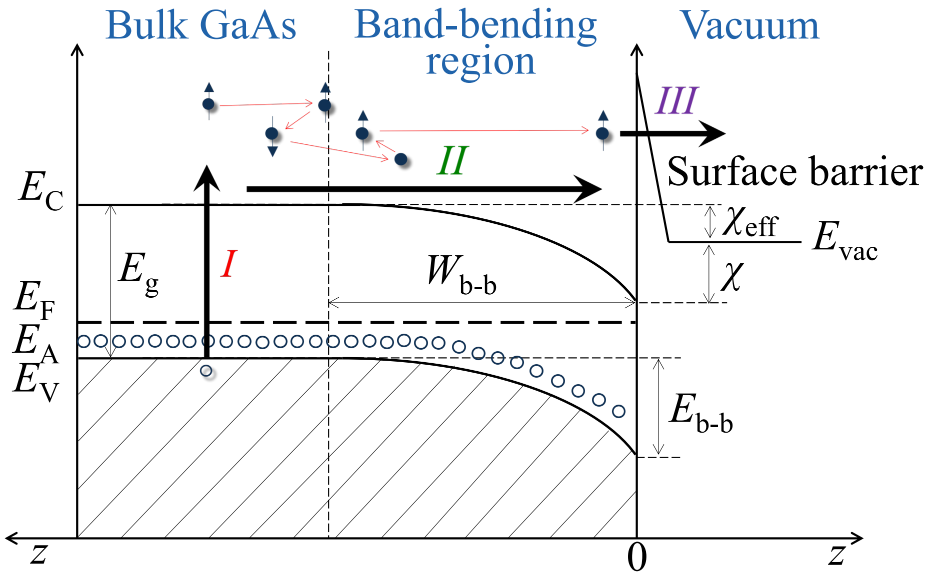
Initial electron distribution in real space



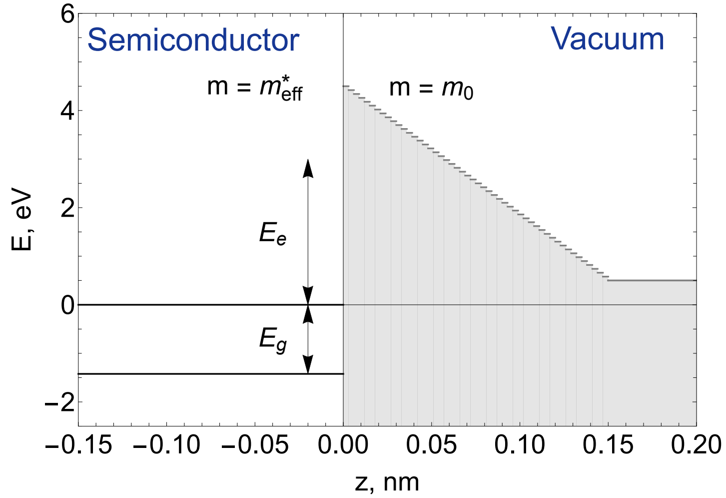
Initial spin orientation of photoexcited electrons

$$ESP_0 = \left|\frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}\right|$$



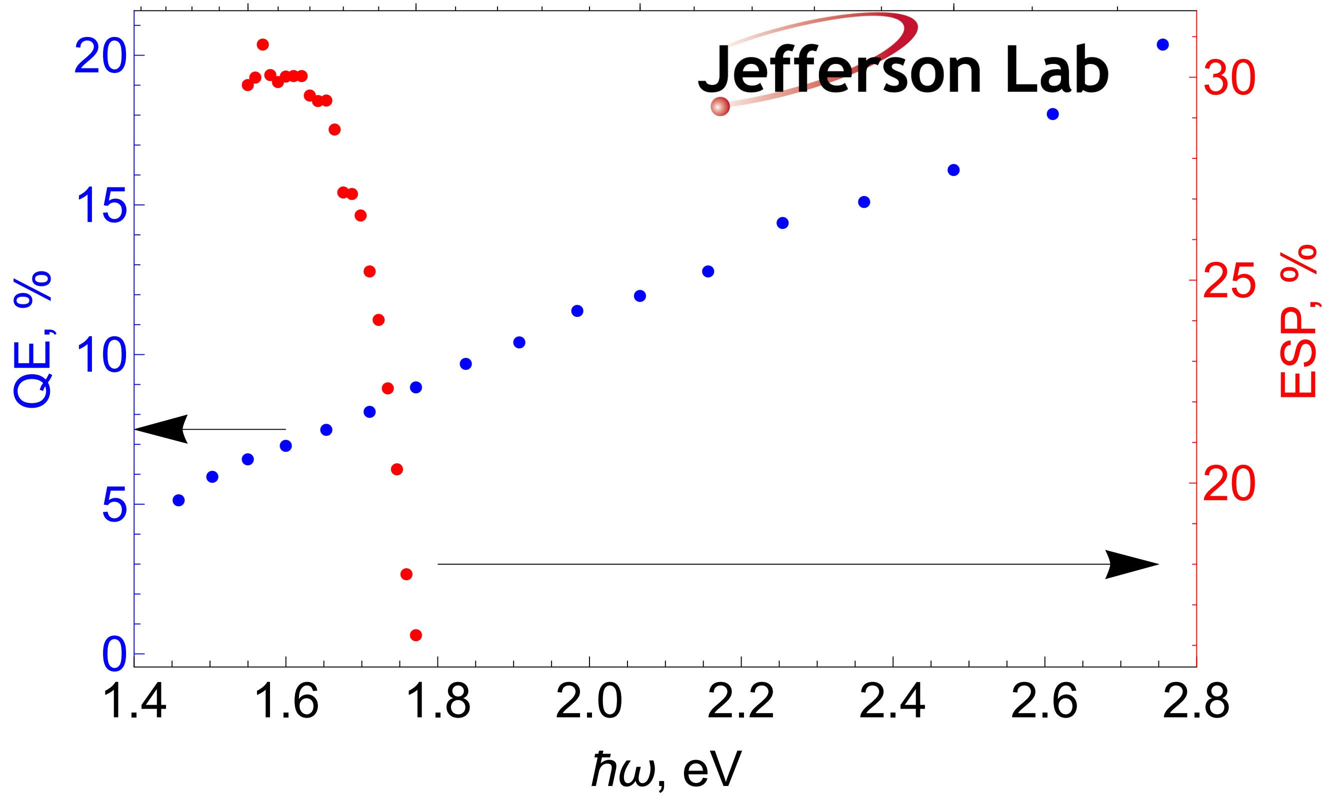


Emission



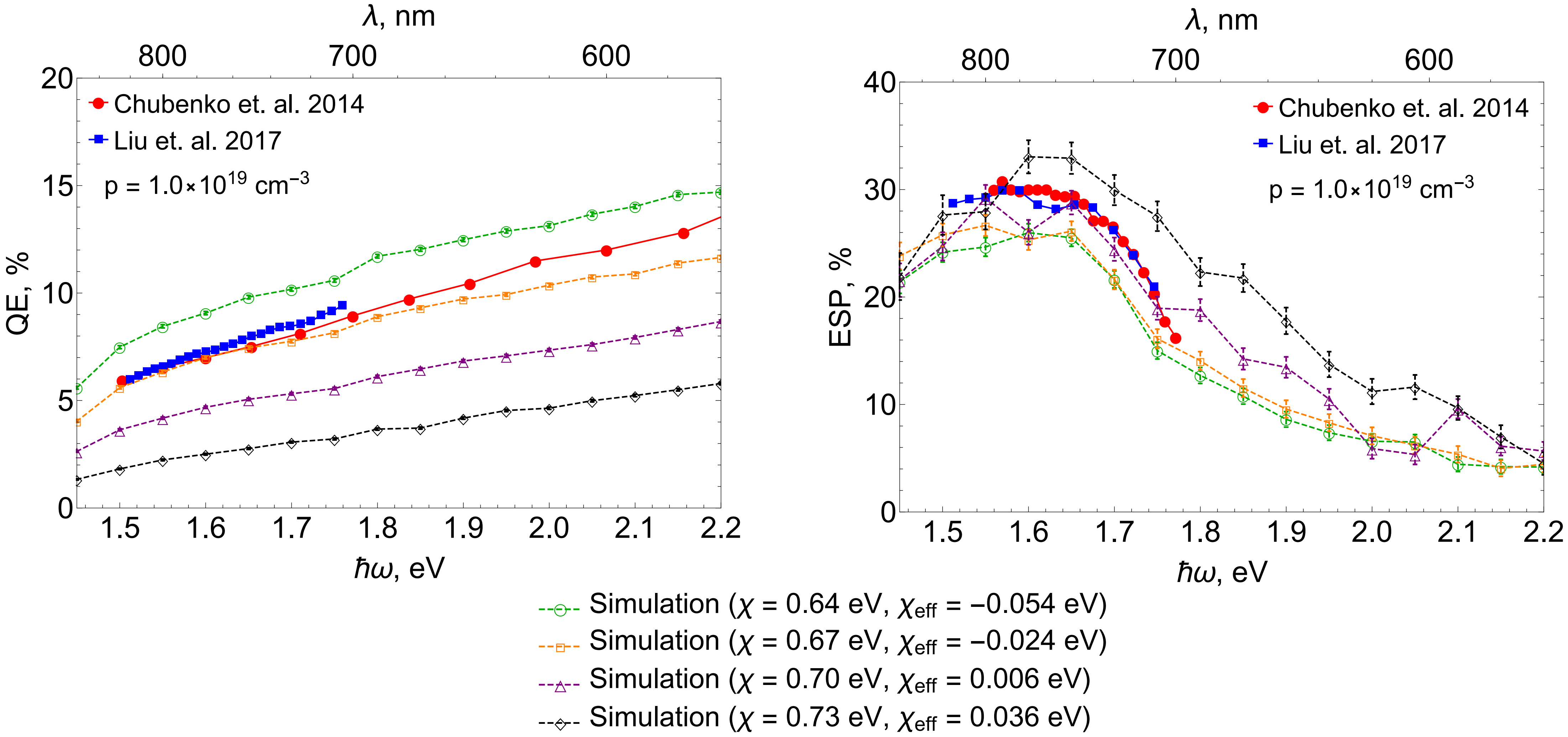
Spin-polarized photoemission from p-type NEA GaAs: I – photoexcitation, II – transport, III – emission.

Monte Carlo study of spin-polarized photoemission from GaAs



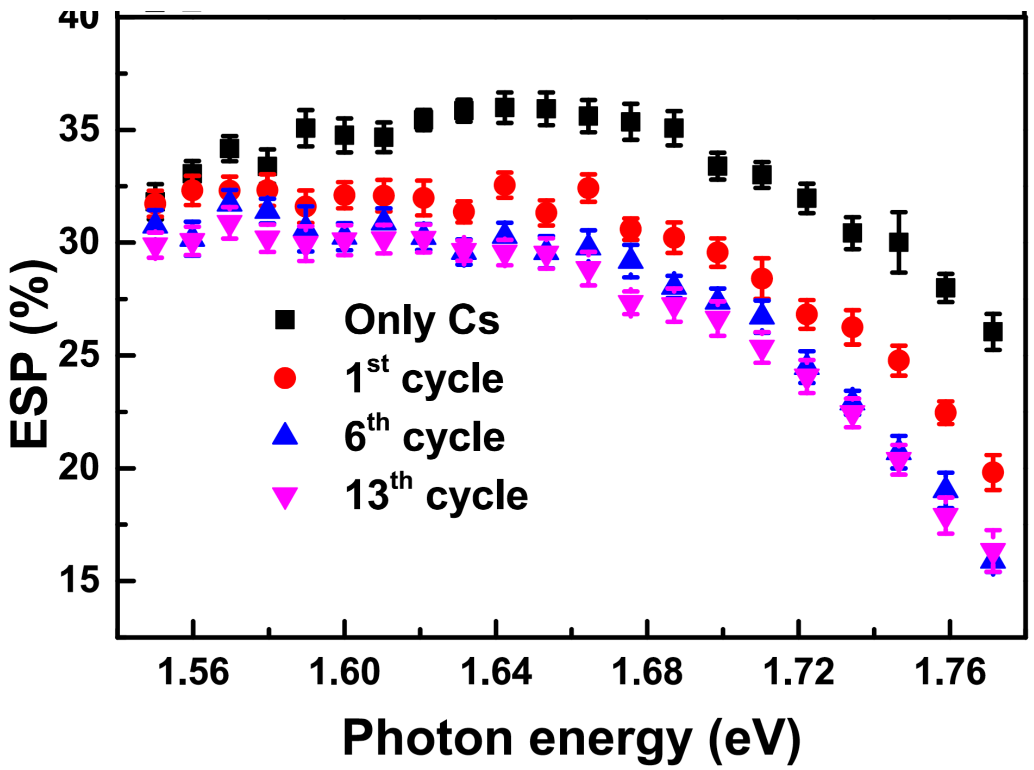
Characteristic behavior of experimental QE and ESP from NEA GaAs.

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

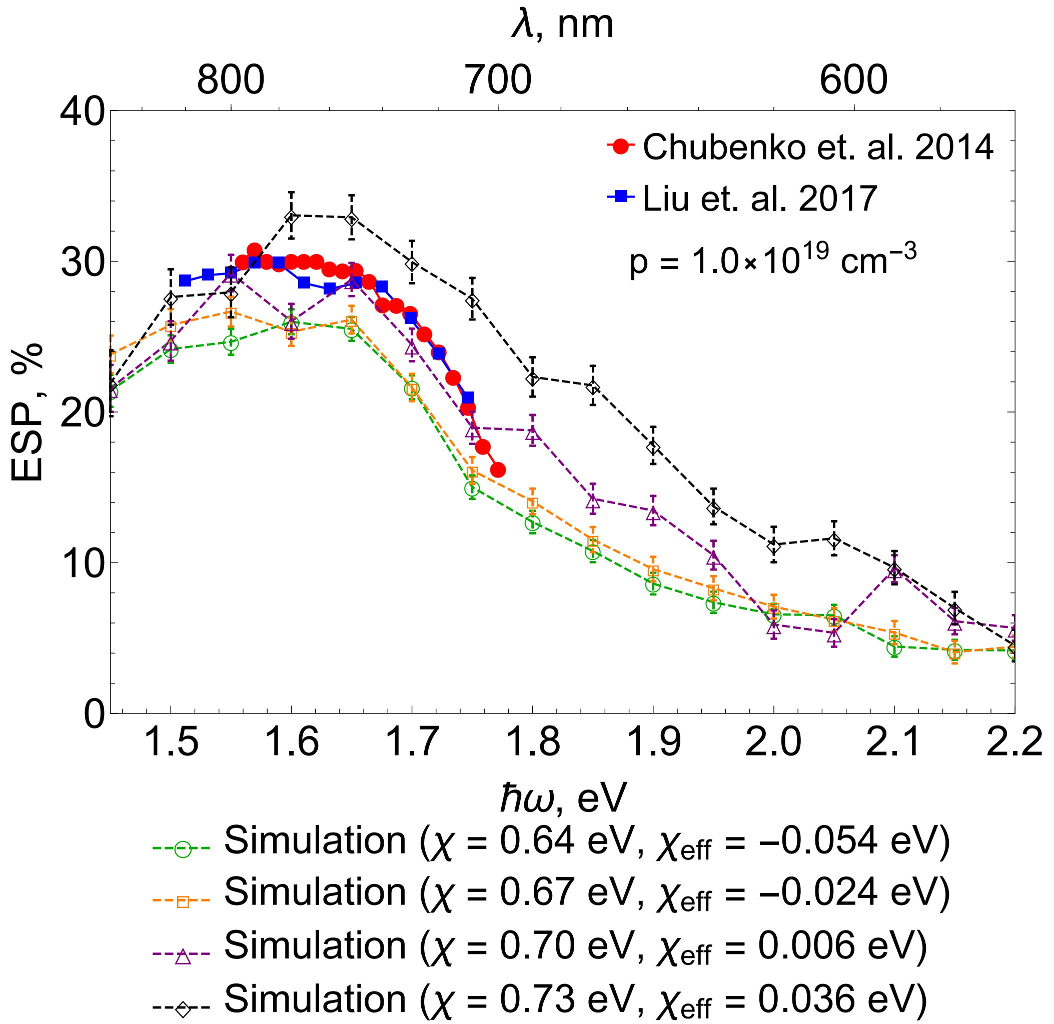


Chubenko et al. J. Appl. Phys. **130**, 063101 (2021)

Monte Carlo study of spin-polarized photoemission from GaAs



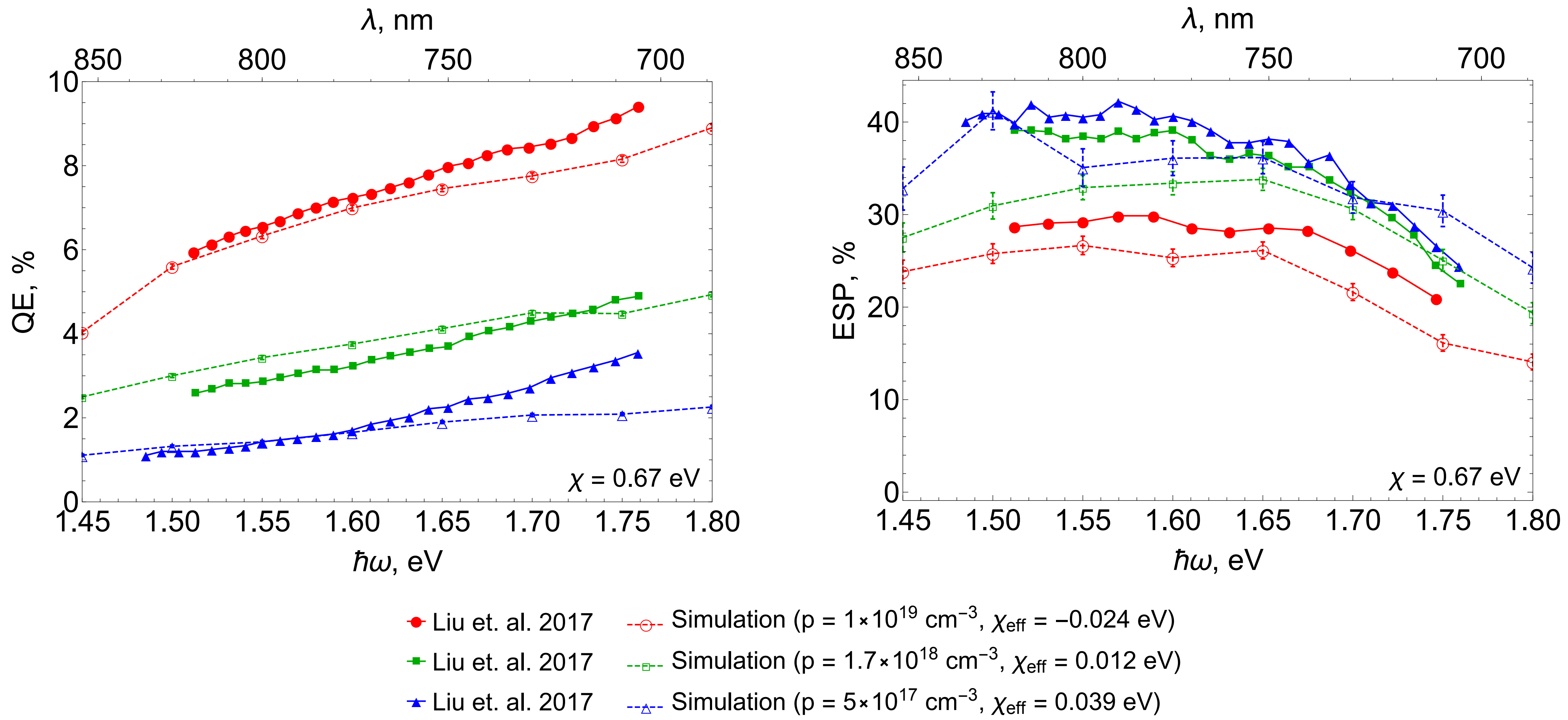
Liu et al. Appl. Phys. **122**, 035703 (2017).



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



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

Future applications of spin-polarized Monte Carlo model

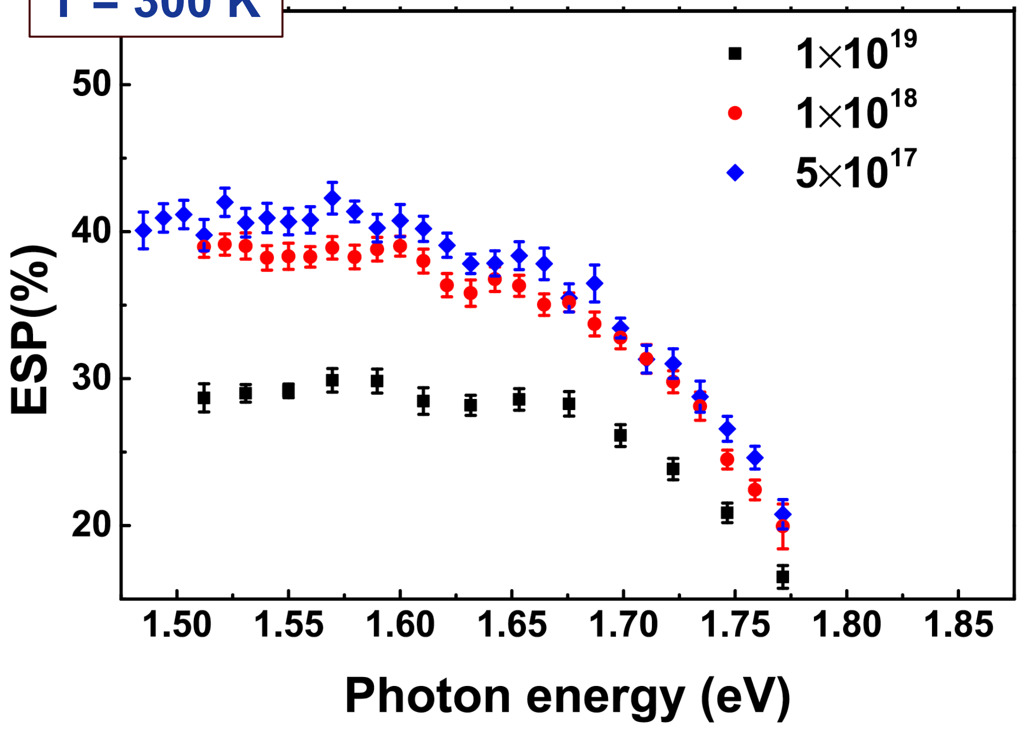
- ✓ Effective/fast modeling of spin-polarized photoemission: C + MPI to run in parallel at HPC cluster.
- ✓ Good agreement with available experimental data.
- ✓ Required model parameters from Density Functional Theory (DFT) calculations.

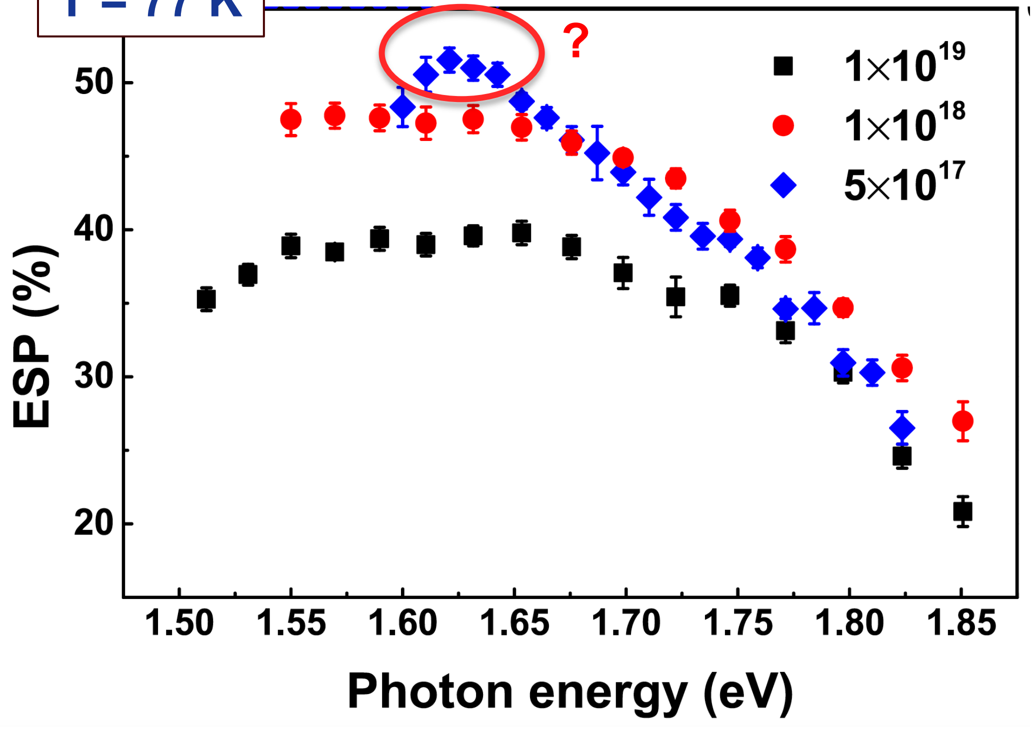
The developed Monte Carlo model establishes a paradigm for future studies of spin-polarized photoemission.

Future applications of spin-polarized Monte Carlo model

Temperature effects on spin-polarized photoemission from bulk GaAs.

$ESP_0 = 50\%$





T = 2 K

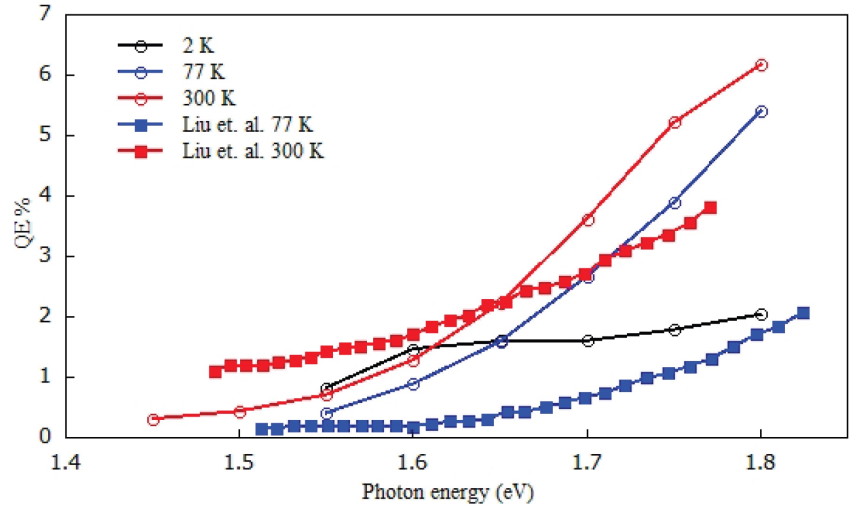
?

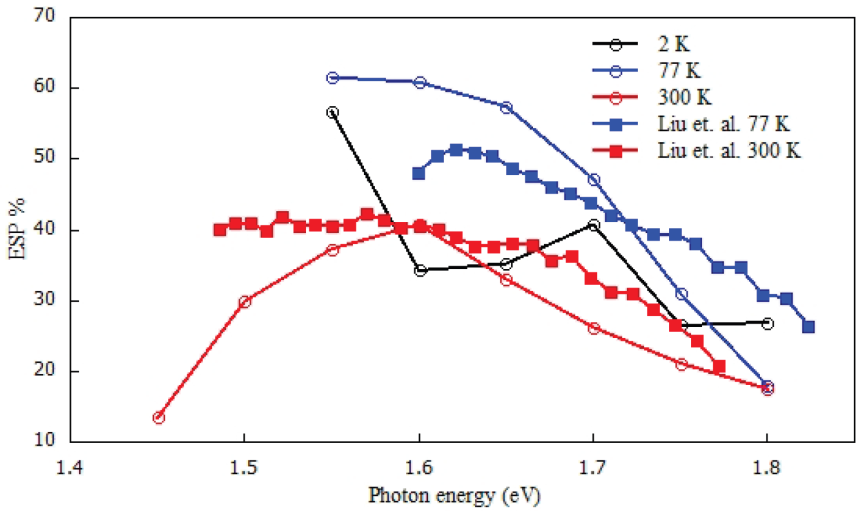
Liu et al. Appl. Phys. 122, 035703 (2017).

Future applications of spin-polarized Monte Carlo model

Preliminary results:

Parameter	2 K	77 K	300 K	Ref. 300 K
Electron's effective mass (m*)				
CB - X	0.294	0.282	0.283	0.58
CB - Γ	0.0687	0.0683	0.0661	0.063
CB - L	0.130	0.130	0.129	0.22
HH	0.368	0.368	0.374	0.50
LH	0.0801	0.0804	0.0785	0.088
SO	0.118	0.117	0.114	0.15
Energy gap (eV)				
Intrinsic	1.52	1.51	1.42	1.42
Split-off	0.362	0.361	0.360	0.332
Splitting energy (eV)				
Γ - L	0.008	0.024	0.034	0.284
Γ - X	0.315	0.330	0.381	0.476
Nonparabolicity factor (eV^{-1})				
Γ	0.571	0.574	0.611	0.61
L	0.498	0.500	0.532	0.461
X	0.328	0.341	0.360	0.204
Optical parameters (ϵ_0)				
H.f. dielectric	11.40	11.43	11.49	10.92
Static dielectric	11.79	11.82	11.90	12.90
Intervalley scattering phonon energy (meV)				
Γ → L	31.8	31.7	29.7	27.8
Γ → X	31.1	30.9	29.7	29.9
L → L	31.8	31.7	29.7	29
L → X	31.5	31.3	29.7	29.3
X → X	31.8	31.7	29.7	29.9
Other				
Polar optical phonon energy (meV)	35.0	34.9	34.1	35.36
Crystal density ($kg \cdot m^{-3}$)	5640	5632	5605	5360
Sound velocity ($m \cdot s^{-1}$)	5127	5125	5004	5240

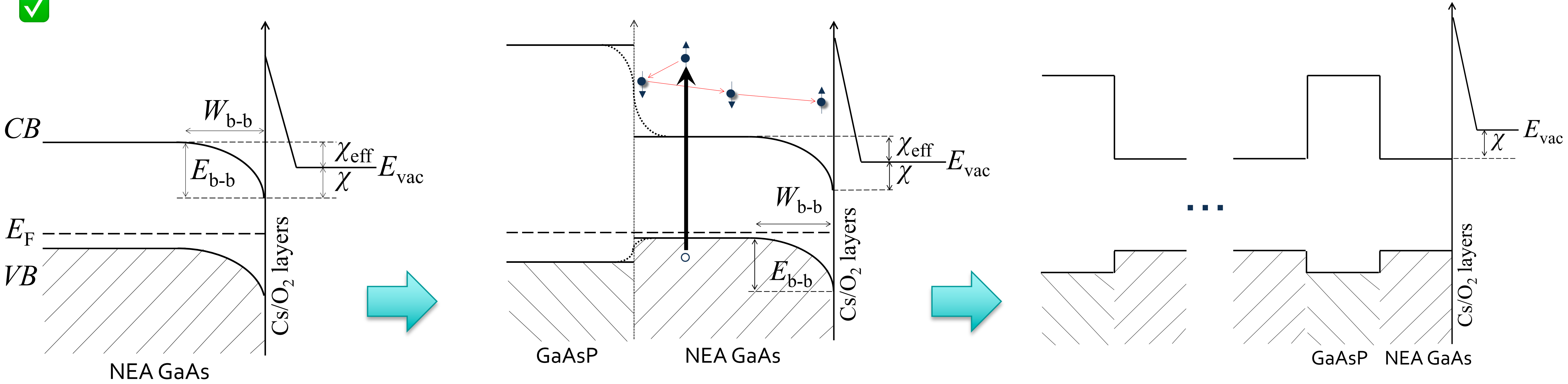




Rodriguez Alicea, Chubenko et al. NAPAC 2022

Spin-polarized photoemission from strained GaAs and Super-Lattice structures.

✅



Future applications of spin-polarized Monte Carlo model

Spin-polarized photoemission from CdTe and other II-VI semiconductors.

	GaAs	CdTe
Direct bandgap	yes	yes
Cs-based activation	yes	yes
Surface quality	high	high
p-doped	yes	yes
Spin-orbit coupling	strong	moderate
Cost	MBE, expensive	ALD, cheap
Accessibility	limited	accessible

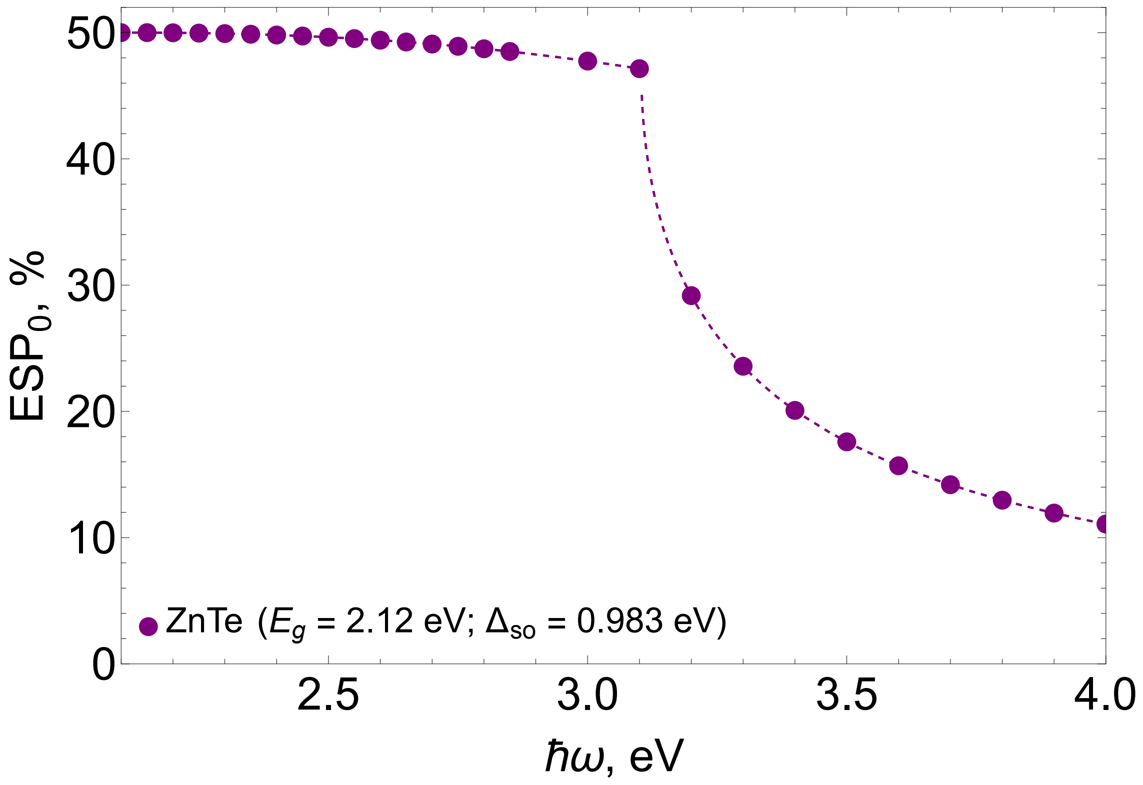
Thursday, October 5

11:05 AM **Cost-effective Atomic Layer Deposition growth of chalcogenide-based polarized electron sources (CdTe, ZnTe, MnTe, etc.)**

Speaker: Dr Harish Bhandari

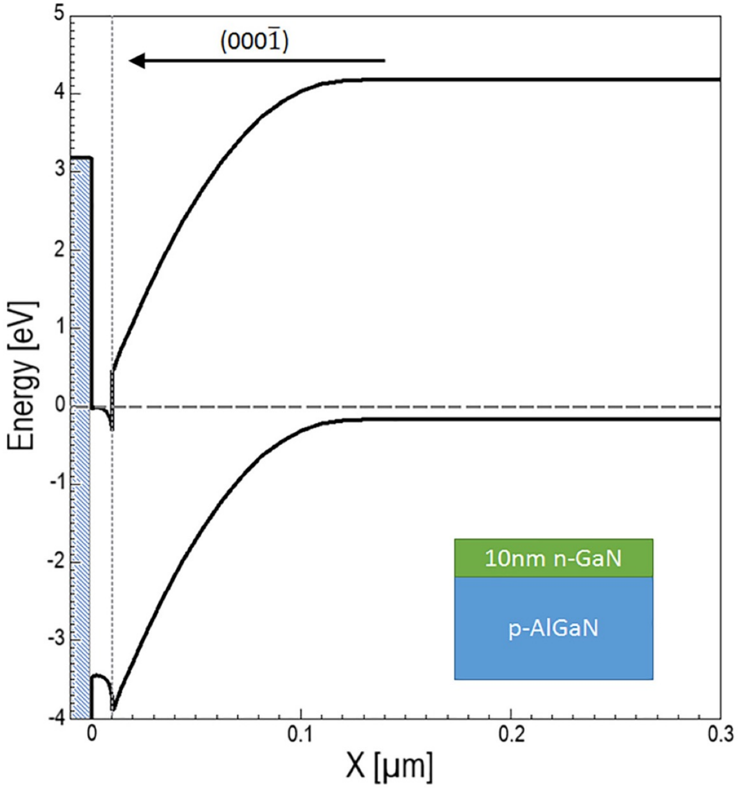
Future applications of spin-polarized Monte Carlo model

Preliminary results for band model parameters available in literature, Boutaiba et al. Phys. REV. B 89, 245308 (2014):



Spin-polarized photoemission from materials with inherently low/negative electron affinity levels.

- Polarization band engineering to achieve an effective NEA condition without the use of Cs at the surface of GaN photocathode structures.
- DFT + Monte Carlo approach to study spin-polarized photoemission from III-Nitride materials.



Marini et al. J. Appl. Phys. 124, 113101 (2018).

Summary and future directions

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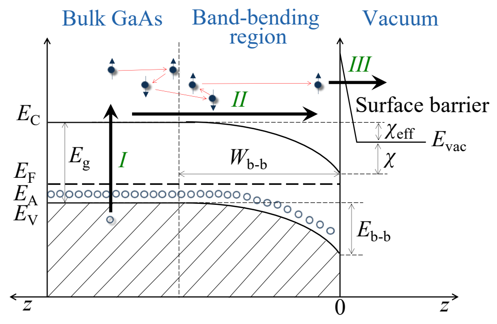
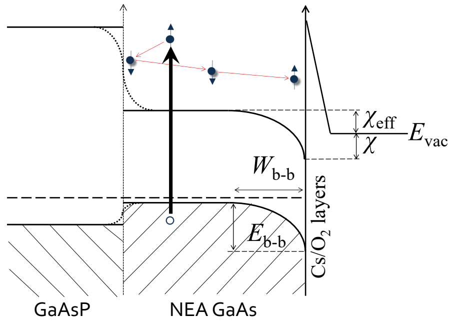
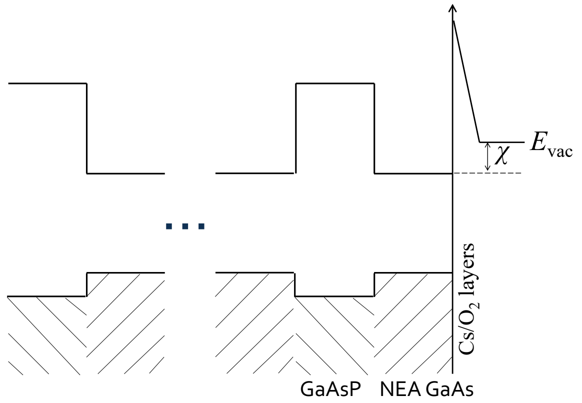
- The detailed Monte Carlo model of photoemission has been developed to model main electron emission characteristics of semiconductor photocathodes. The model provides good agreement with experimental data for bulk NEA GaAs at room temperature. ✅



- The work in progress to implement both low temperature and lattice strained adjustments to the Monte Carlo Approach using DFT results.



- The developed Monte Carlo model will be modified further to study spin-polarized photoemission from novel materials and layered structures.



Acknowledgements

John Callahan (NIU)
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Luca Cultrera (BNL)
Ivan Bazarov (Cornell University)
Andrei Afanasev (GWU)

Thank you!