Pushing the limit of photodetection by bandgap engineering through alloying and stacking

Shiva Abbaszadeh

Radiological Instrumentation Laboratory

Electrical and Computer Engineering

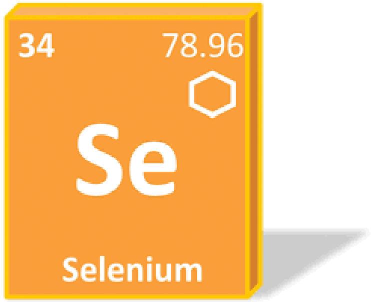
ril.soe.ucsc.edu

UC SANTA CRUZ | Baskin Engineering

Outline

1. Why Selenium?
2. Alloying selenium
3. Device configuration
4. Summarize key Takeaways
5. Future Directions & Research Opportunities

Amorphous Selenium



www.hruimetal.com

Selenium is part of the **chalcogen group** (Group VI) in the periodic table.

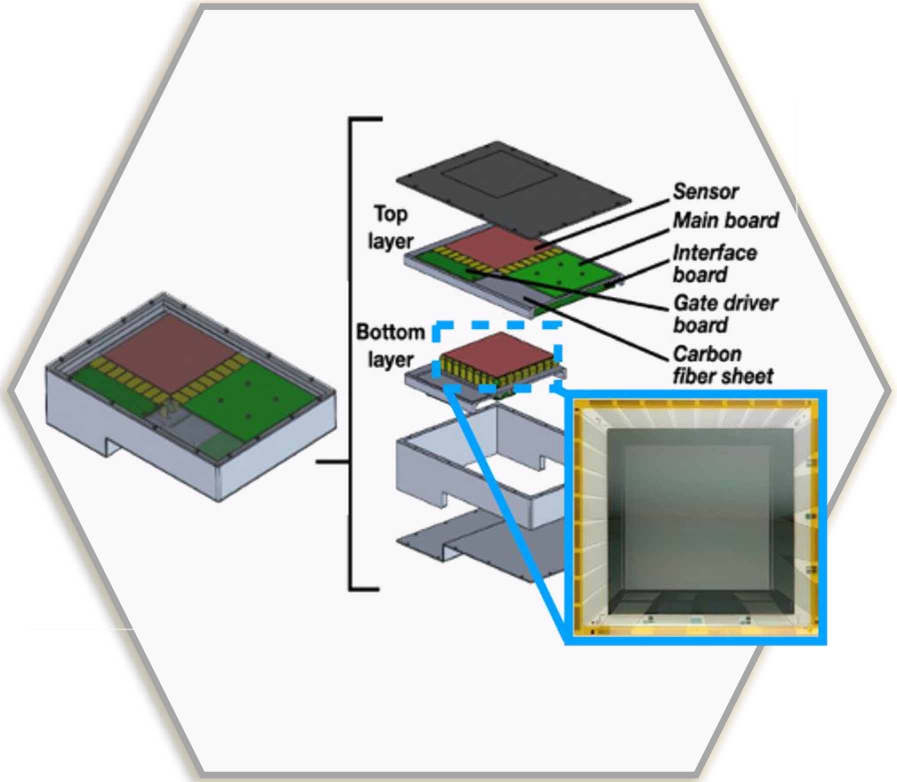
Amorphous selenium is widely used in **X-ray detectors.**

Benefits:

- Large area, low cost, maturity
- Good absorption properties for relatively low energy (mammography, 30kVp), 200 µm thick layer
- Low dark current ($E_g = 2.2$eV)
- **Potential for gain (avalanche)**
- High spatial resolution (direct detector)

Kasap, *et al.* *J Mater Sci: Mater Electron* **26**, 4644–4658 (2015)

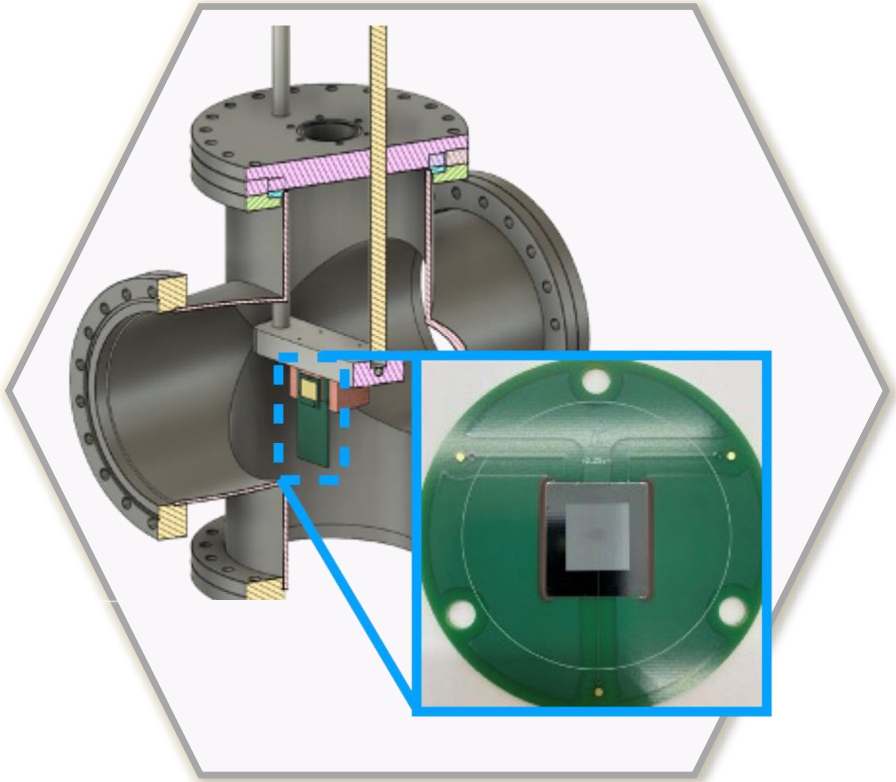
From Medical Imaging to High Energy Physics



a-Se flat panel detector

W. Zhao et al, *Medical Physics* 30, 254-263 (2003)

Hellier et al, SPIE Medical Imaging (2023)

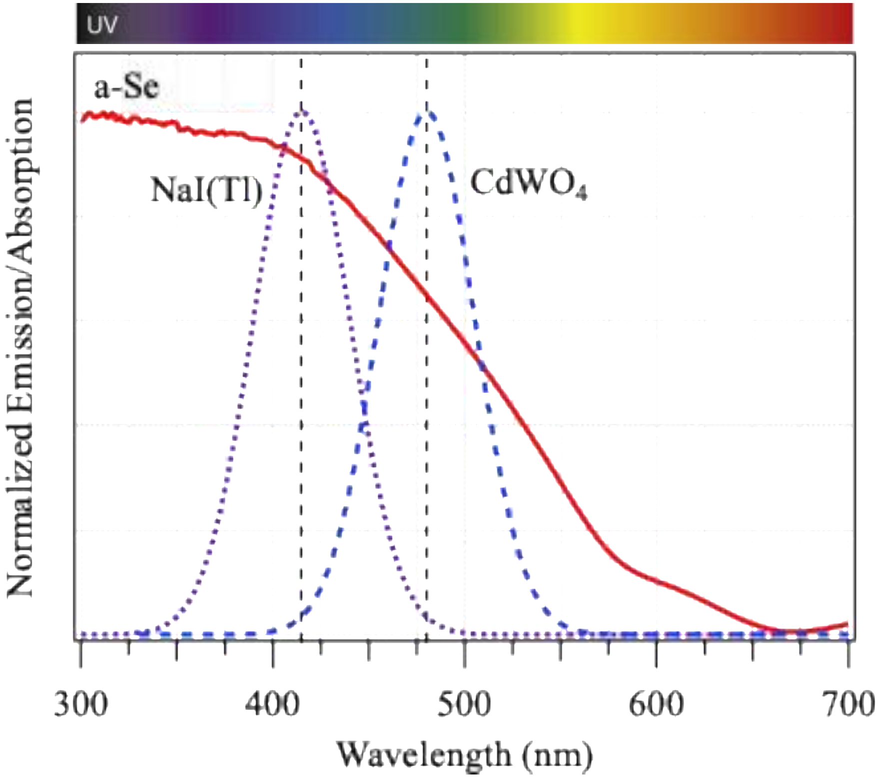


a-Se detector for use in liquid noble detector

Rooks, M., et al, *Journal of Instrumentation* 18, P01029 (2023).

A-Se as Indirect Conversion:
Pushing the Limits of Sensitivity

Matching Sensitivity Spectrum of Photodetector with Emission of Scintillator

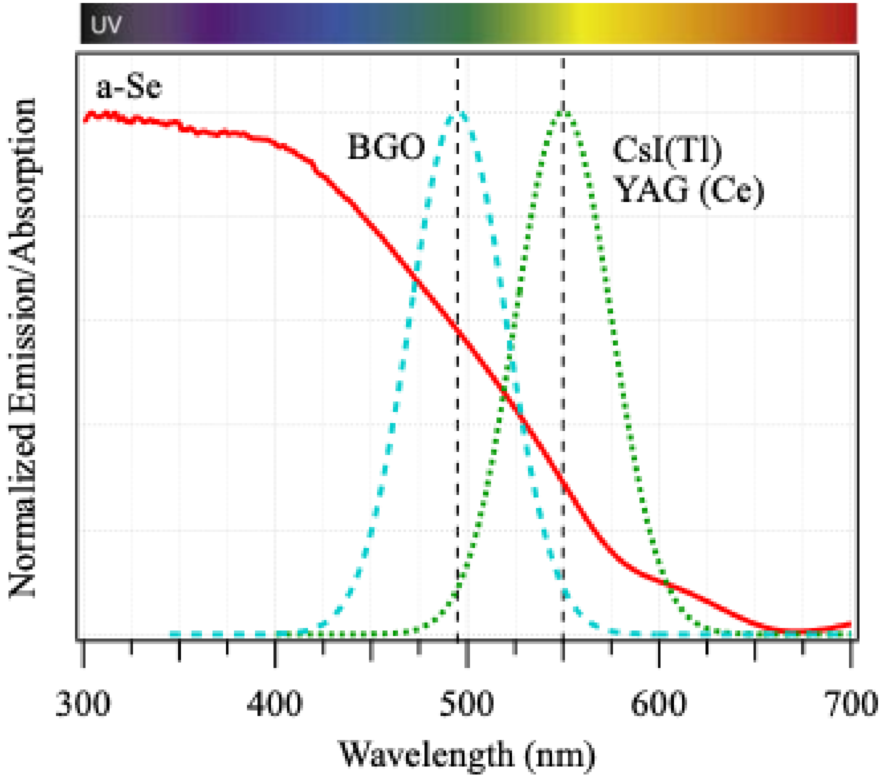


a-Se is an excellent absorber for VUV-UV-Blue emitters like liquid Ar, NaI, undoped CsI.

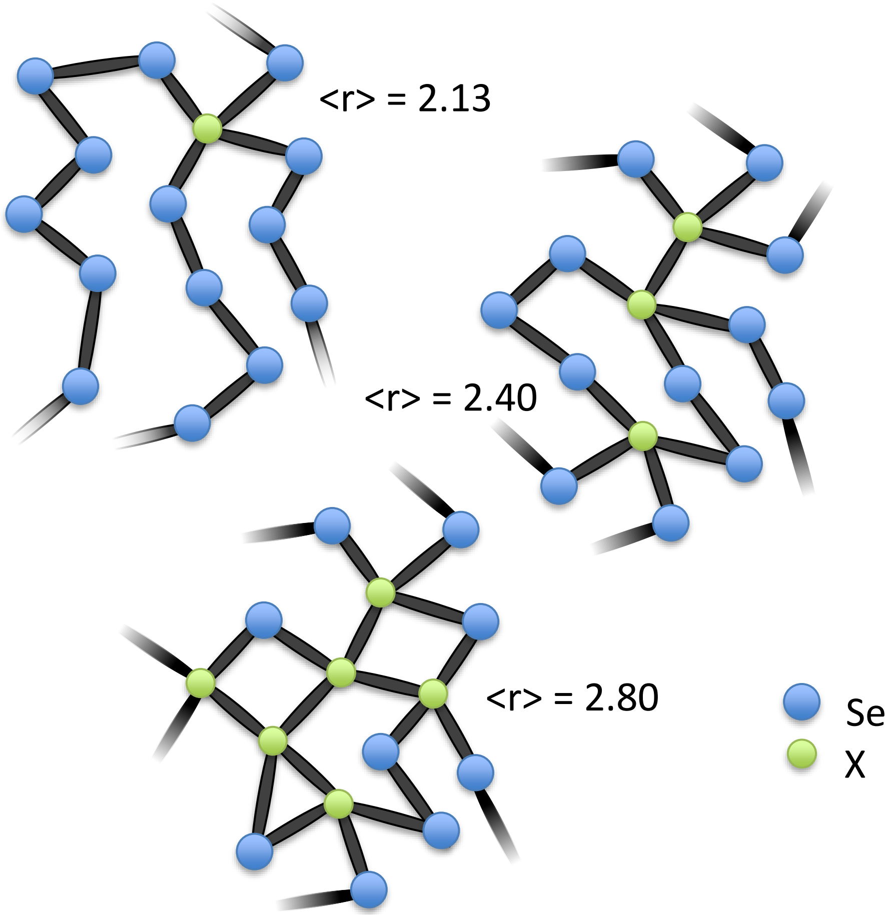
A-Se as Indirect Conversion:
Pushing the Limit of Sensitivity

Matching Sensitivity Spectrum of Photodetector with Emission of Scintillator

But has low absorption – and low efficiency – for high-yield long-wavelength emitters



Doping and Alloying with Group IV, V, & VI elements



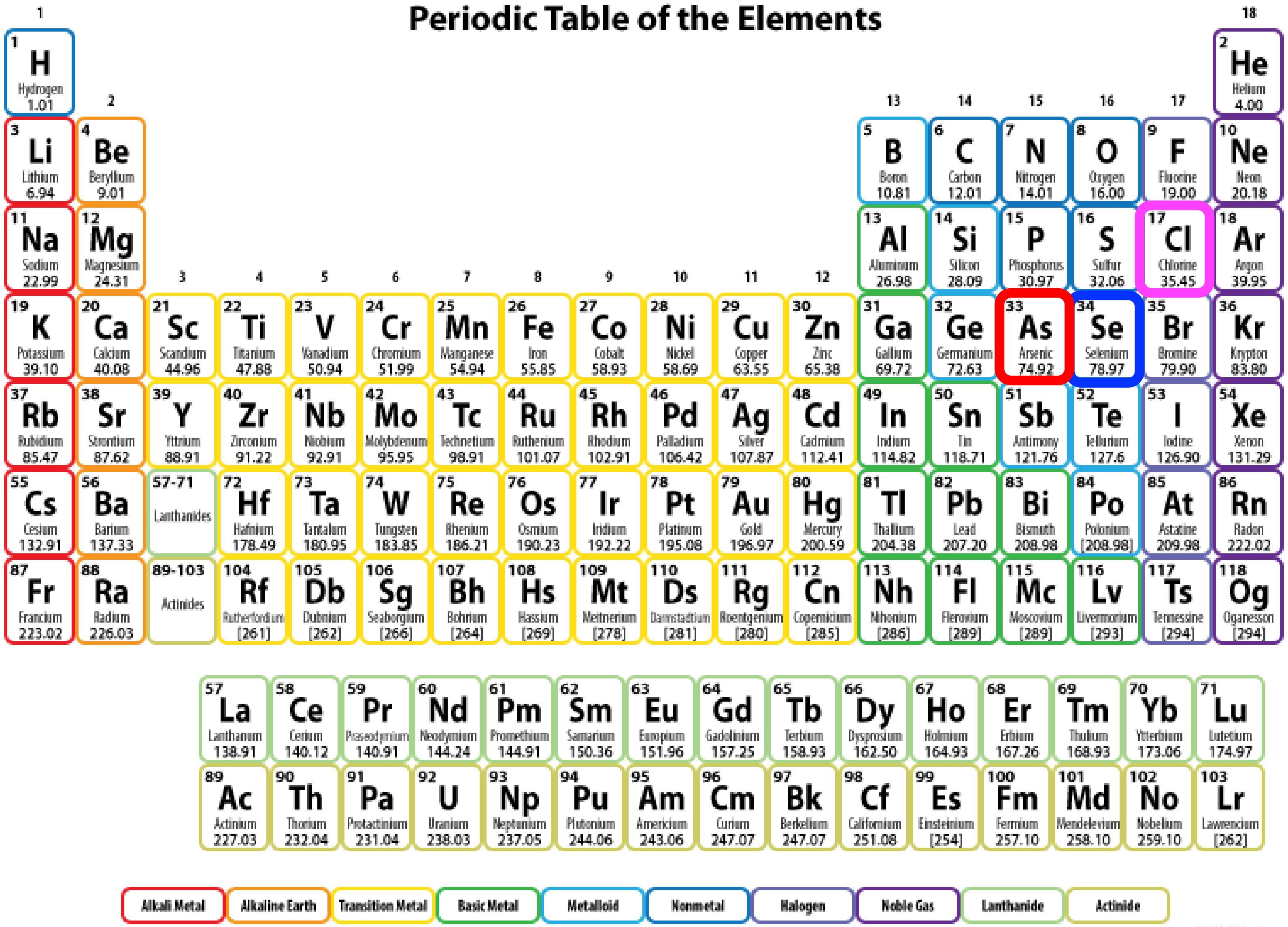
Can change properties such as:

- Band gap
- Leakage currents
- Carrier transport
- Sensitivity
- Structure & coordination
- Crystallization
- Stability

Doping and Alloying with Group IV, V, & VI elements

Arsenic

- Doped at 0.1 – 0.5 %
- Stabilizes, preventing crystallization
- Introduces deep hole trap states, lowering carrier lifetime



Chlorine

- 10-40 ppm
- Mitigates deep hole traps from As
- Improves carrier lifetimes, with minimal effect on mobilities

Kasap et. al, *JMS Mat. in Elec.* (2000), v 11, 3, p 179

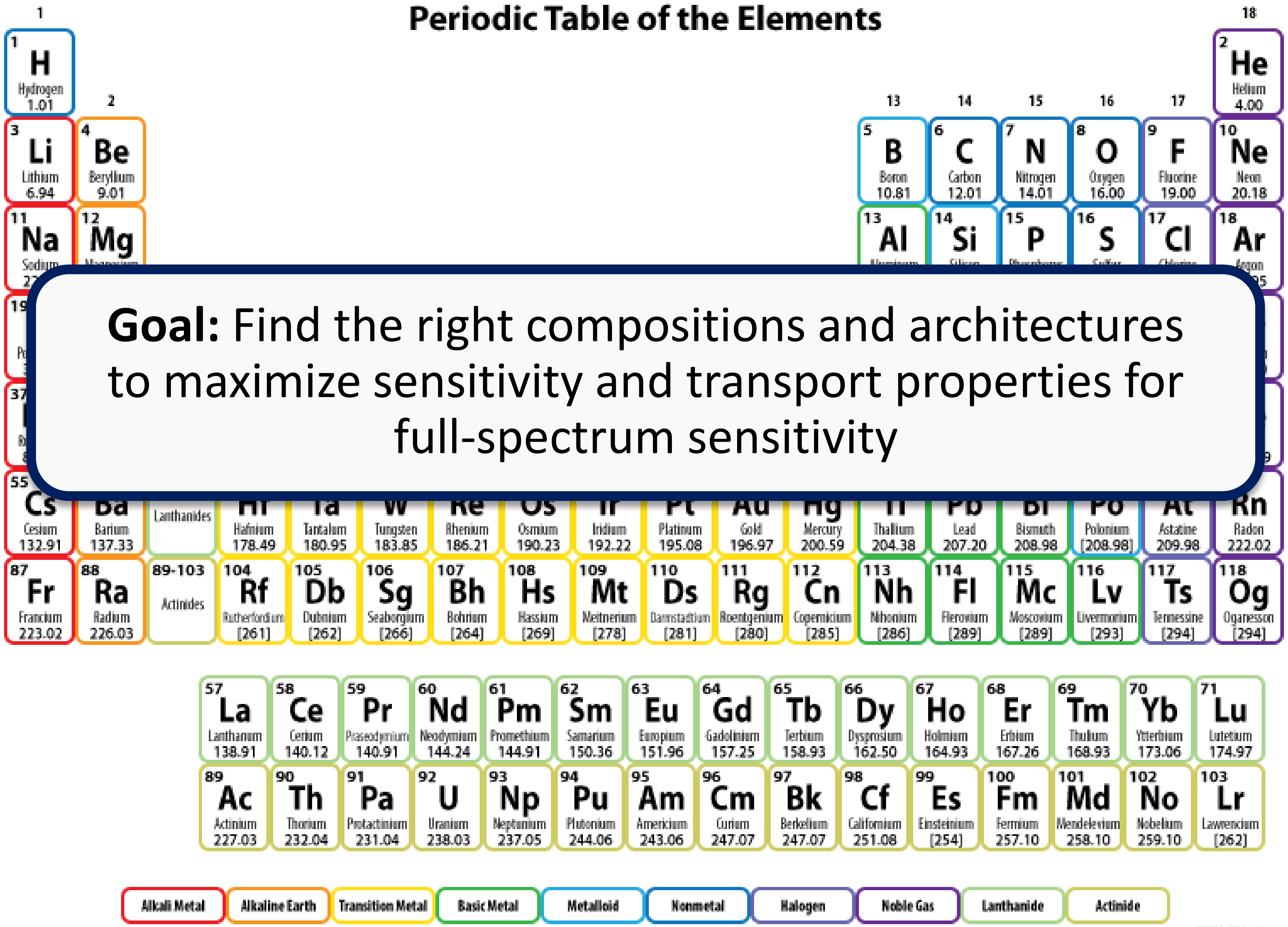
Kasap et. al, *Semiconductors*, (2003) v 37, 7, p 789

Doping and Alloying with Group IV, V, & VI elements

Tellurium

- Increasing Te decreases E_g
- Induces traps, lowering μ and τ
- Increases conductivity
- Increases crystallization temperature

Hellier et. al, *ACS AEM* (2023), v 5, 5, p 2678



Goal: Find the right compositions and architectures to maximize sensitivity and transport properties for full-spectrum sensitivity

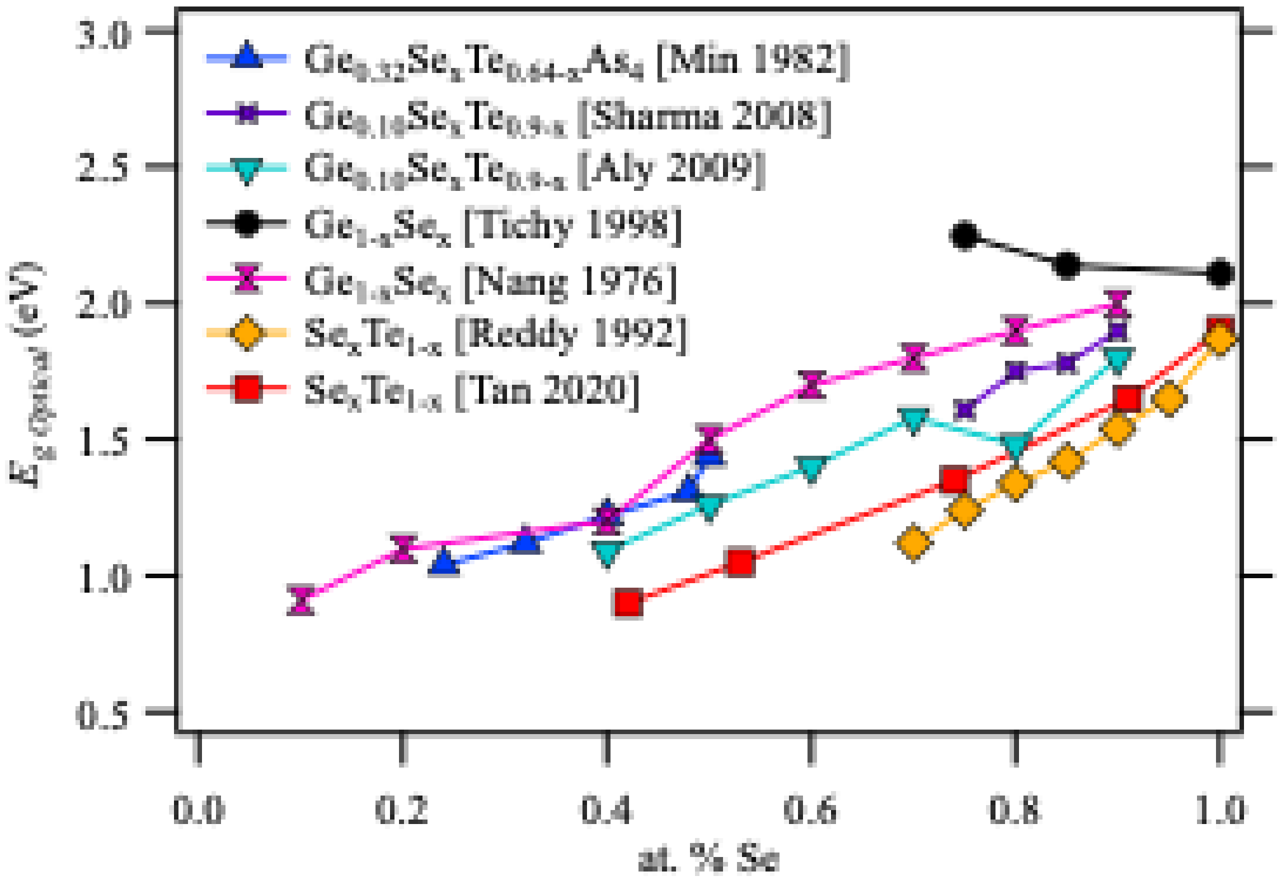
Germanium

- Ge may lower E_g, however studies differ
- Lowers μ_e, then increases
- Increases thermal stability
- Properties are very content dependent

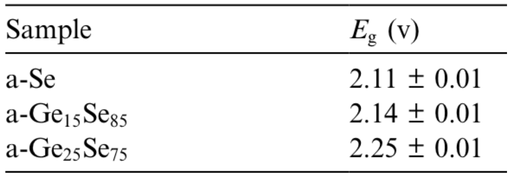
Nang, et al., *Jpn. JAP* (1976), v 15, 5, p 849

Kim & Shirafuji, *Jap. JAP.* (1978), v 17, 10, p 1789

Doping and Alloying with Group IV, V, & VI elements



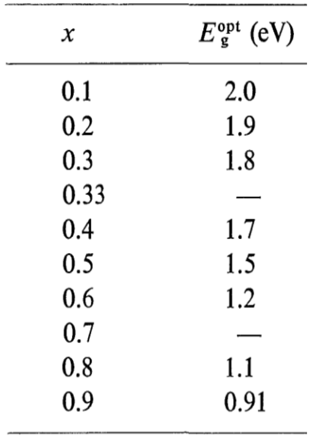
- Se-Te previously investigated for photodetection, solar cells, memory applications
- Ge-Se & Ge-Se-Te primarily investigated for switching devices, memory
  - ➢ Literature reaches differing conclusions on optical and electronic properties, **leaving questions waiting to be answered**



Sample	E_g (v)
a-Se	2.11 ± 0.01
a-$Ge_{15}Se_{85}$	2.14 ± 0.01
a-$Ge_{25}Se_{75}$	2.25 ± 0.01

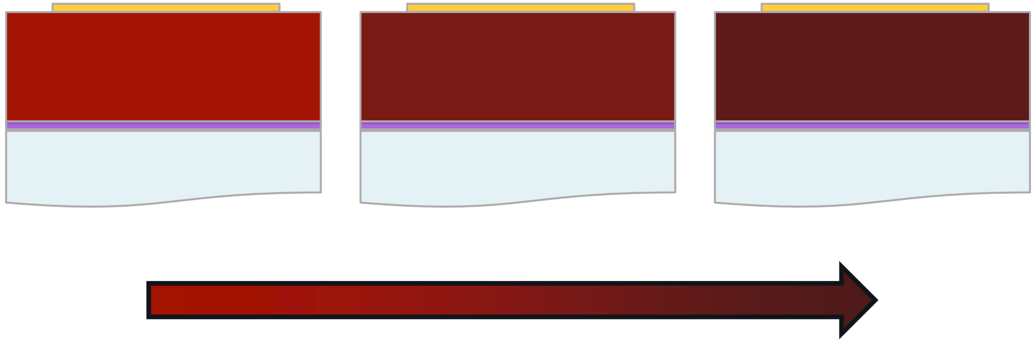
L. Tichy, et al., *J. Non-Cryst. Sol*. (1998), v 240, 1, p 177

T. T. Nang, et al., *Jpn. J. Appl. Phys.*(1976), v 15, 5, p. 849



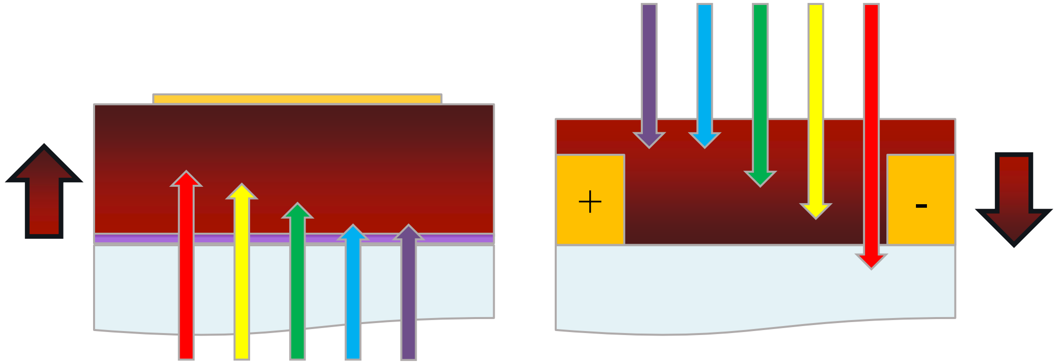
x	E_g^{opt} (eV)
0.1	2.0
0.2	1.9
0.3	1.8
0.33	—
0.4	1.7
0.5	1.5
0.6	1.2
0.7	—
0.8	1.1
0.9	0.91

Exploring Se-Te Concentration and Stacked Configurations



Se-Te Photodetectors for long wavelength sensitivity

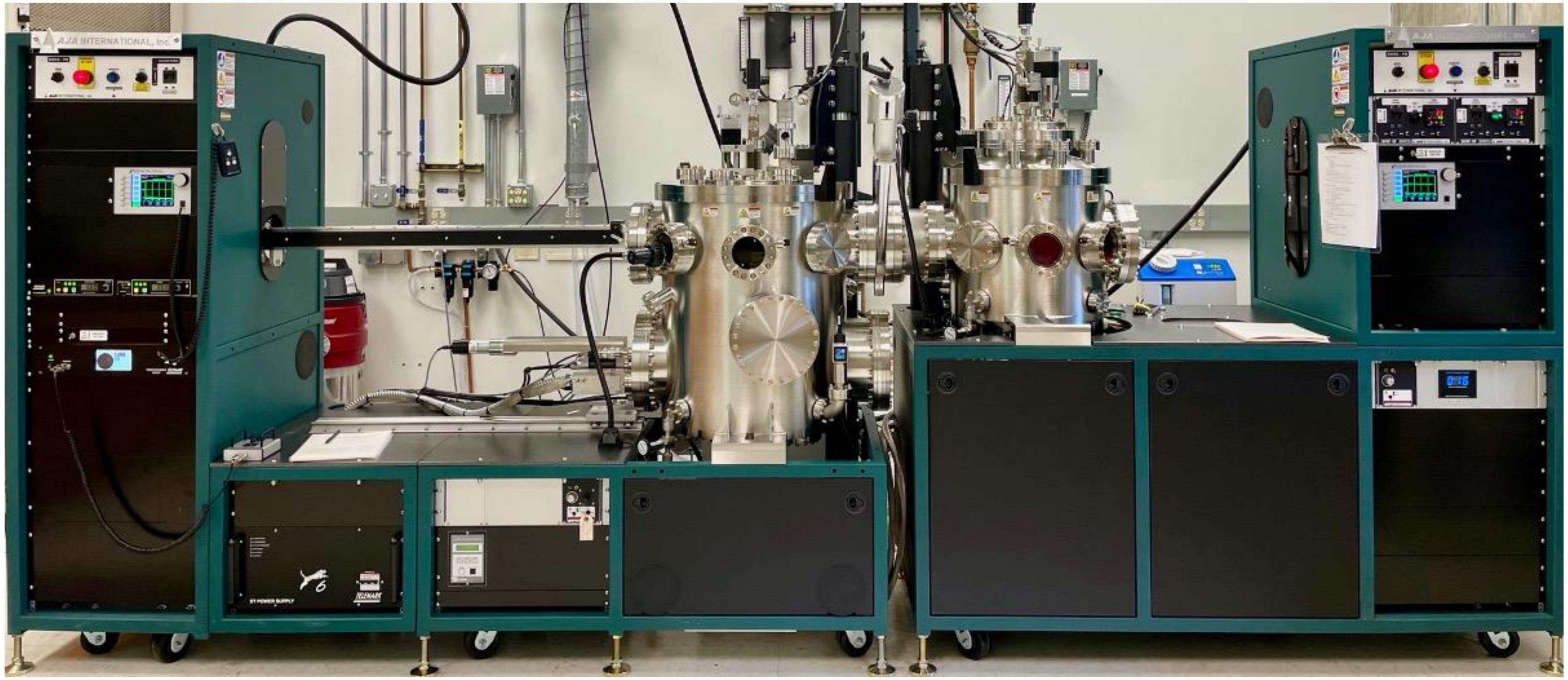
1. Develop Se-Te fabrication capabilities
2. Investigate and confirm optical and electronic properties



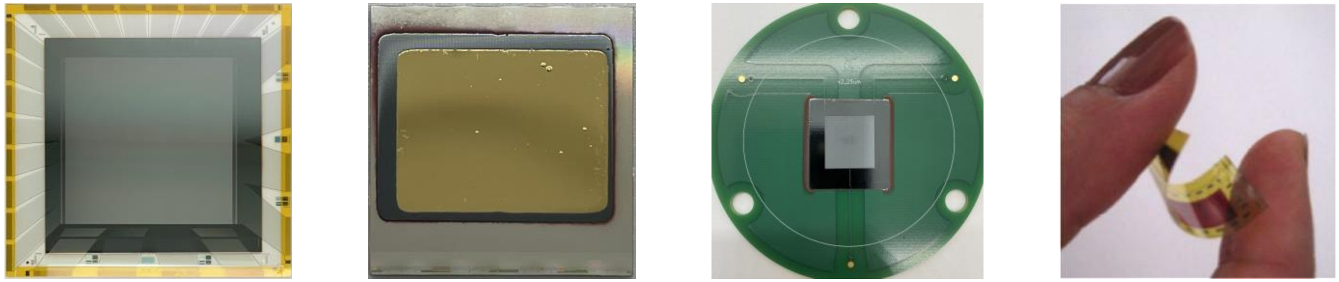
Stacked Se/Se-Te for high transport and full spectrum sensitivity

1. Fabricate stacked architectures of Se/Se-Te in vertical and lateral structures
2. Compare optoelectronic properties to determine optimum architectures

RIL Fabrication Facilities



- Custom-built, dedicated selenium thermal evaporator and e-beam deposition systems
- Capable of multi-material depositions, including all layers for detector architecture



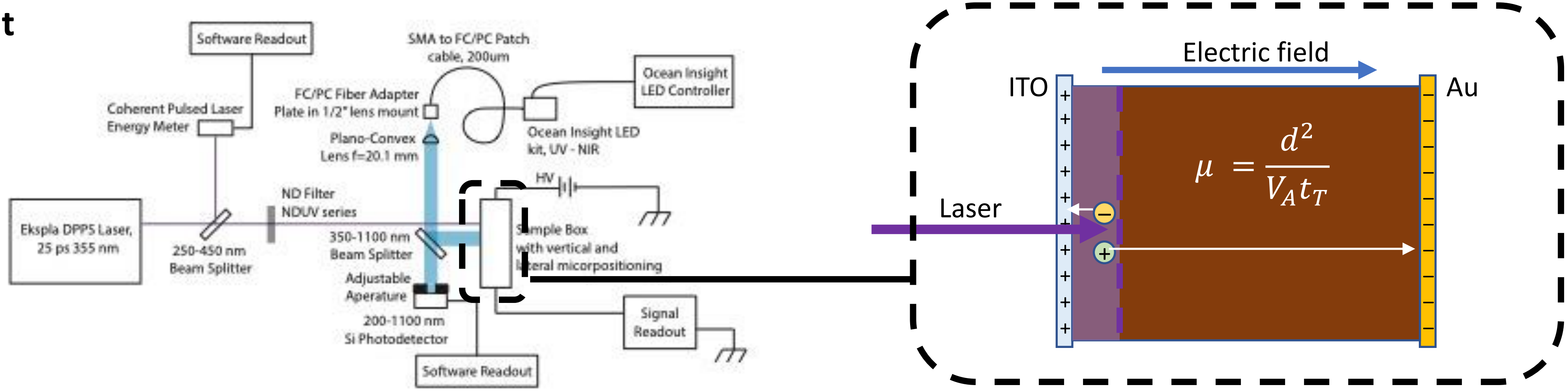
Dr. Kaitlin Hellier
Postdoctoral Scholar

Hamid Mirzanezhad
PhD student

Molly McGrath
MS student

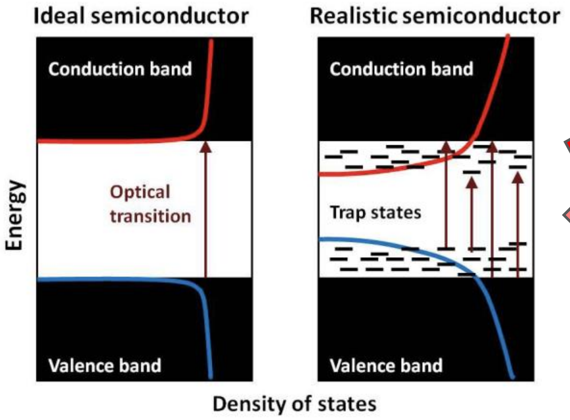
Characterization

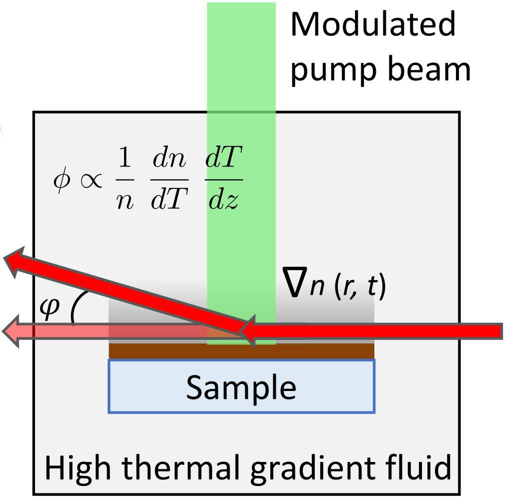
Transient Photocurrent Time of Flight & Dark/Photocurrent



$$\mu = \frac{d^2}{V_A t_T}$$

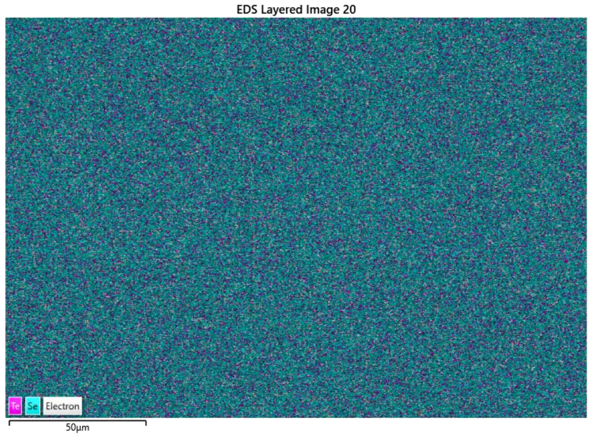
Photothermal Deflection Spectroscopy



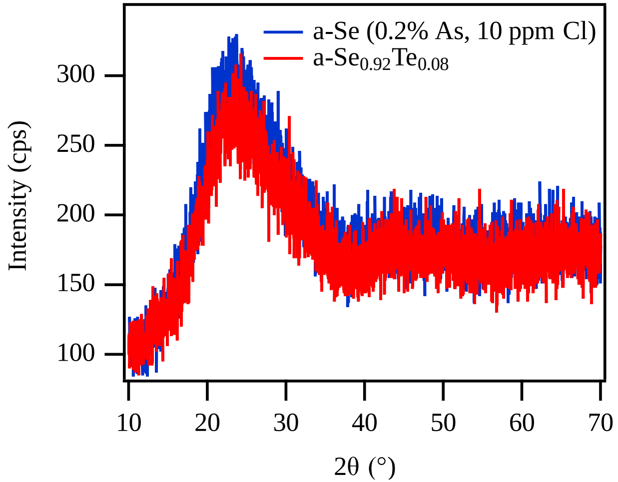


$$\phi \propto \frac{1}{n}\,\frac{dn}{dT}\,\frac{dT}{dz}$$

SEM-EDS Mapping



X-ray Diffraction

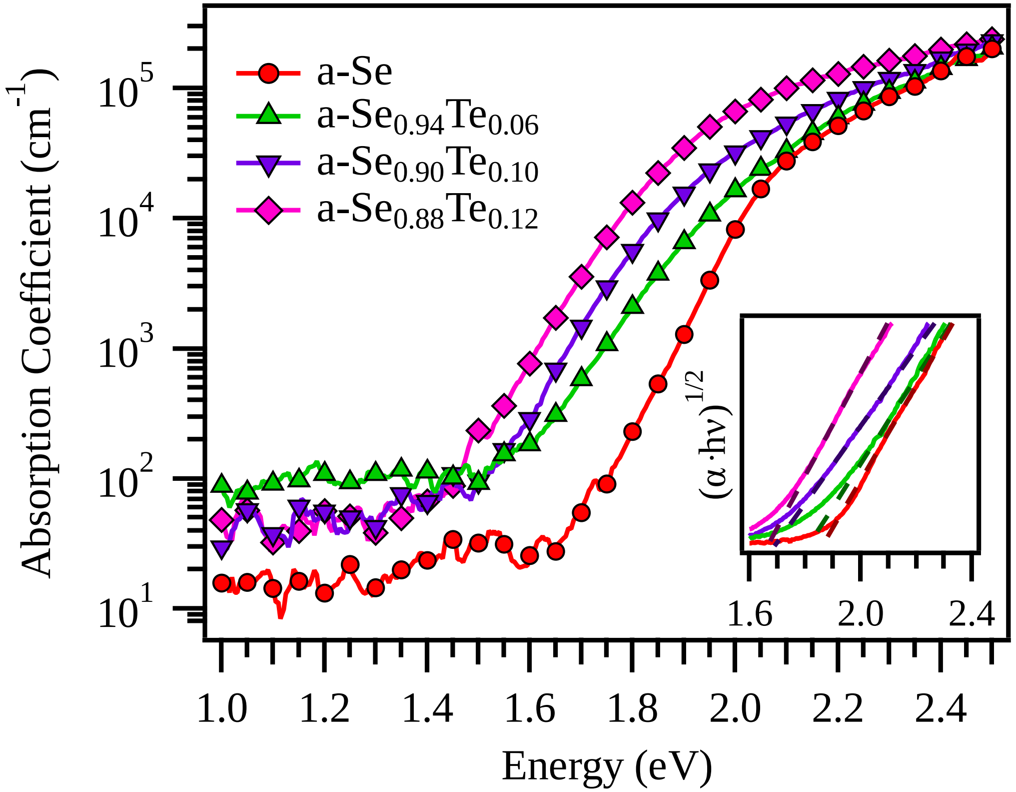


Alloying of a-$Se_{1-x}Te_x$

Increasing Te Content

Hellier et. al, *ACS AEM* (2023), v 5, 5, p 2678

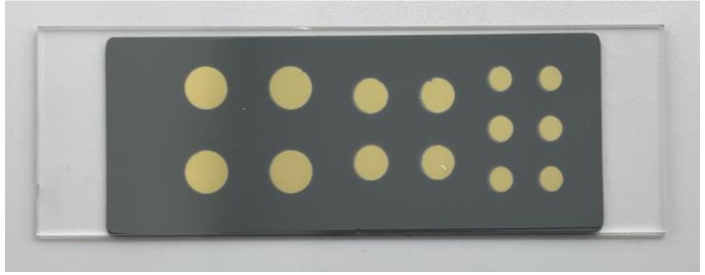
Photothermal Deflection Spectroscopy

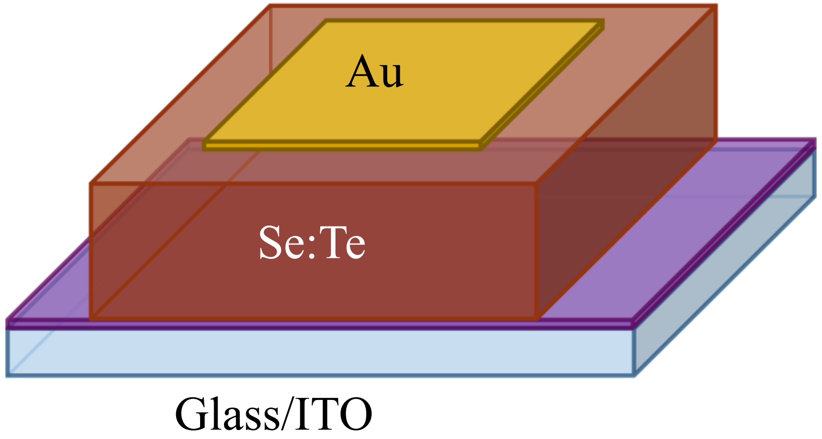


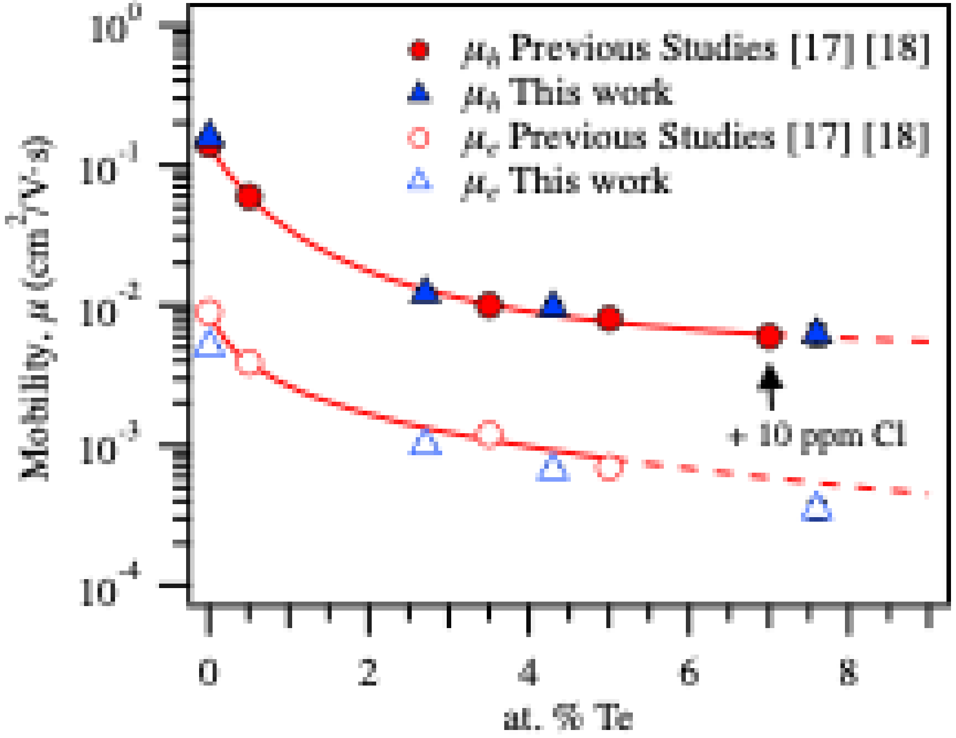
Hellier et. al, *ACS AEM* (2023), v 5, 5, p 2678

Alloying of a-$Se_{1-x}Te_x$

a-$Se_{0.90}Te_{0.10}$ sample





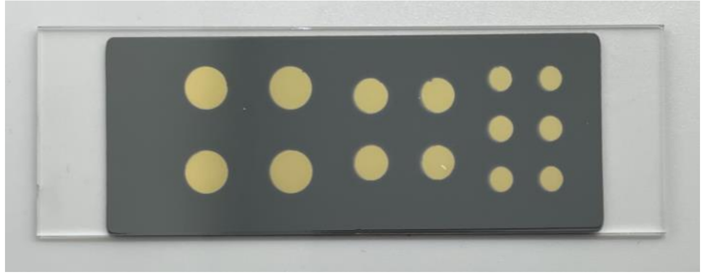


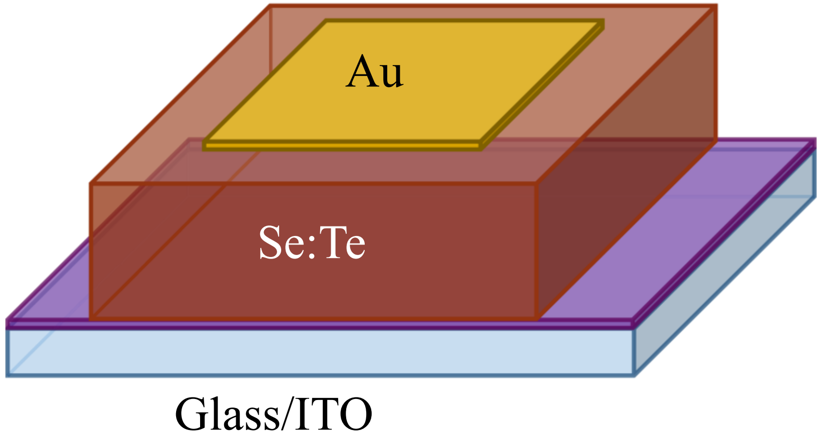
[17] Kasap and Juhasz, *J.Non-Cryst. Sol.* (1985), v 72, 1, p 23
[18] *Juhasz et a., J. Mat. Sci.* (1987), v 22, 7, p 2569

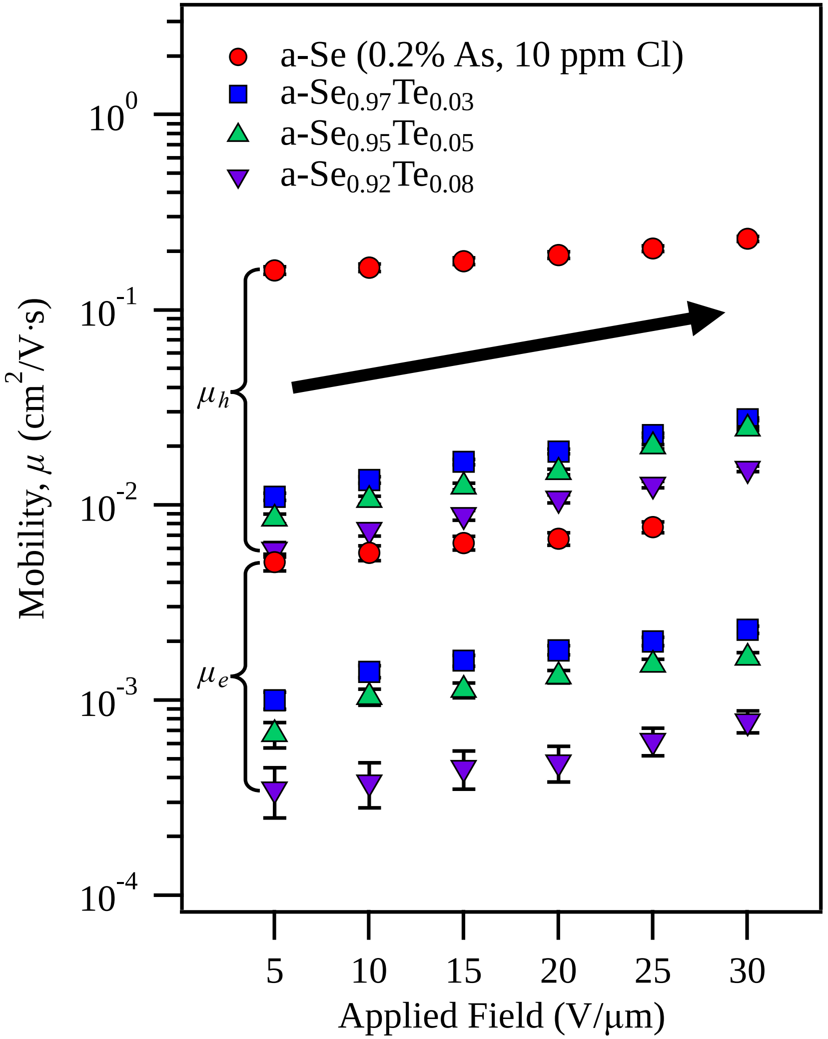
Hellier et. al, *ACS AEM* (2023), v 5, 5, p 2678

Alloying of a-$Se_{1-x}Te_x$

a-$Se_{0.90}Te_{0.10}$ sample

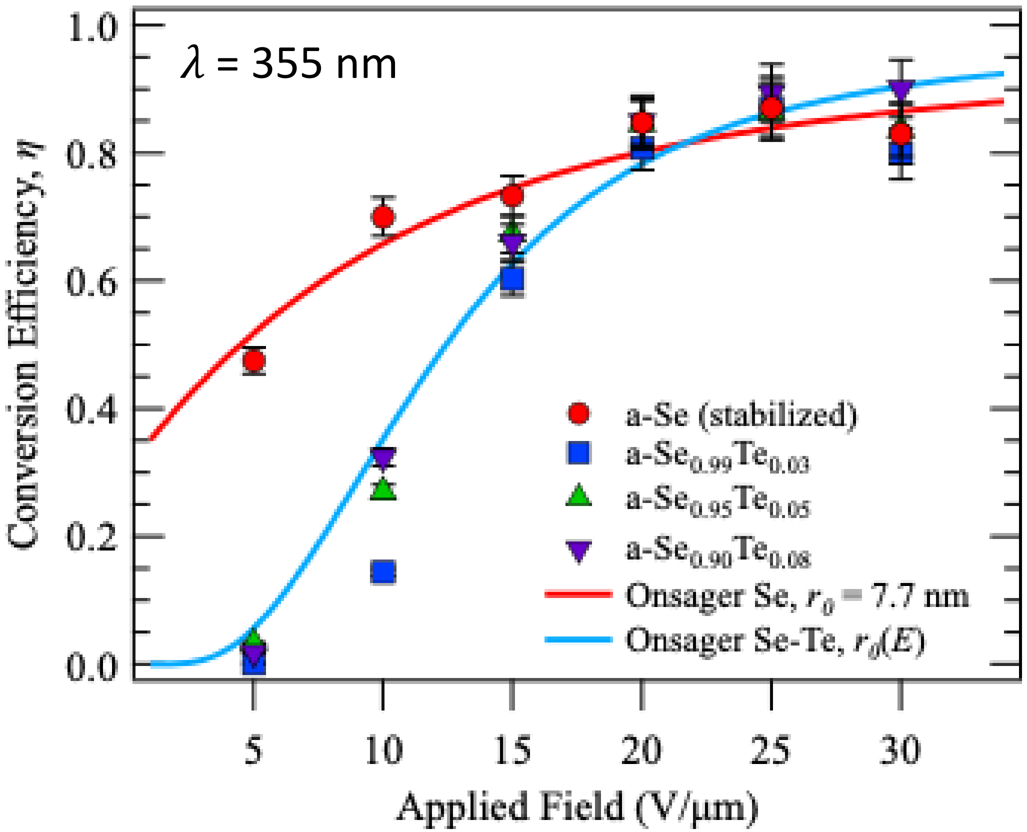






Hellier et. al, *ACS AEM* (2023), v 5, 5, p 2678

Alloying of a-$Se_{1-x}Te_x$



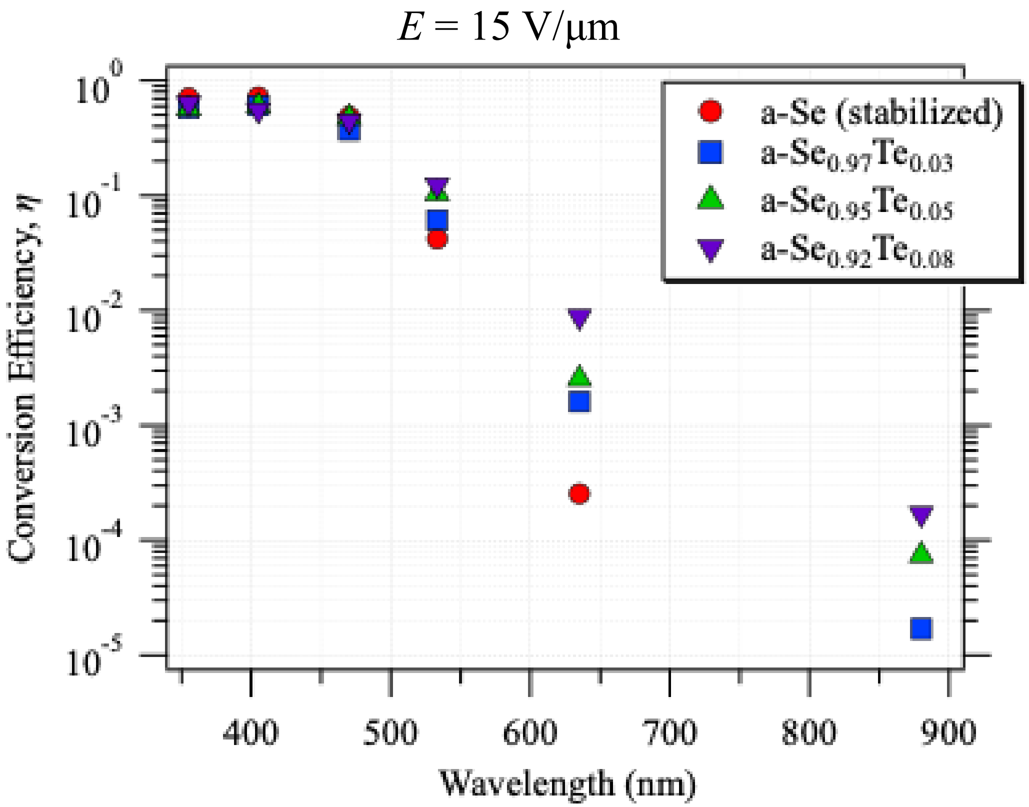
- At low fields, CE limited by trap states and low thermalization
- At moderate to high fields, CE recovers as carriers gain enough energy to escape traps

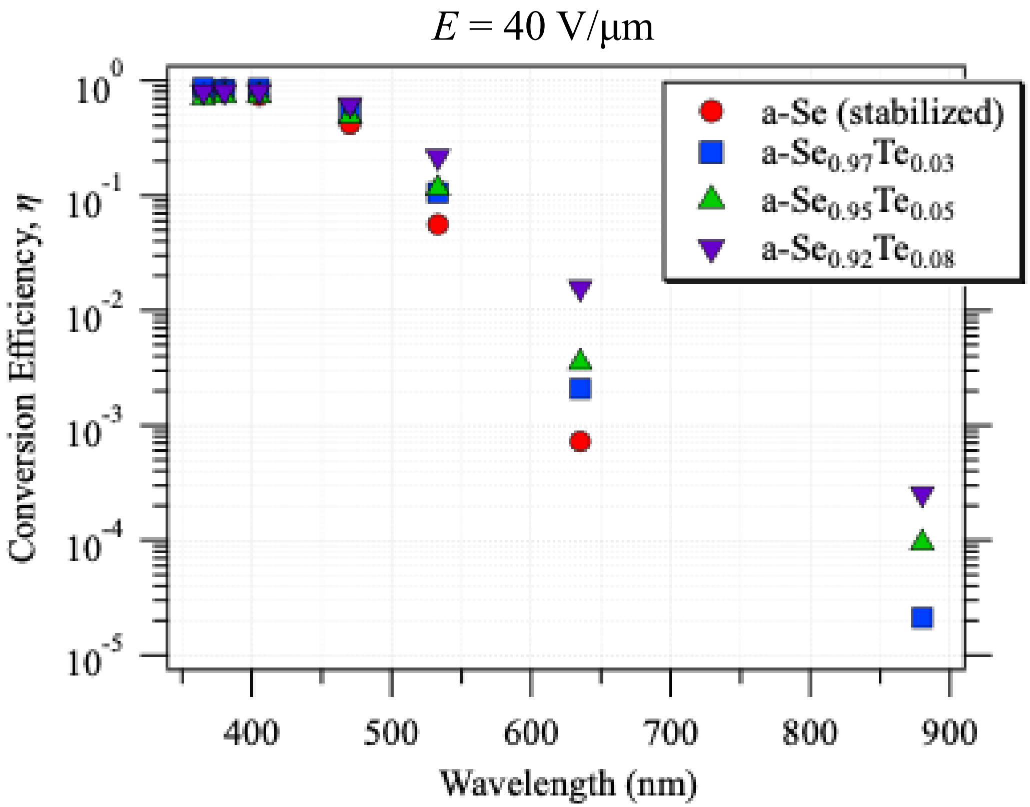
→ Modified Onsager model, with thermalization length (r_0) a function of field – not just wavelength

Hellier et. al, *ACS AEM* (2023), v 5, 5, p 2678

Pai and Enck, *Phys. Rev. B* (1975), v 11, 12, p

Alloying of a-$Se_{1-x}Te_x$

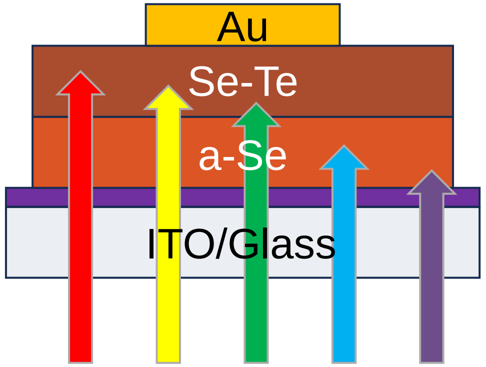


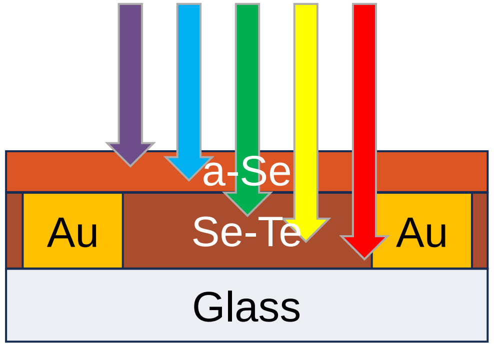


Increasing Te concentration → increased CE at long wavelengths, especially at higher fields

Hellier et. al, *ACS AEM (*2023), v 5, 5, p 2678

Stacked a-Se/Se-Te for Improved Sensitivity





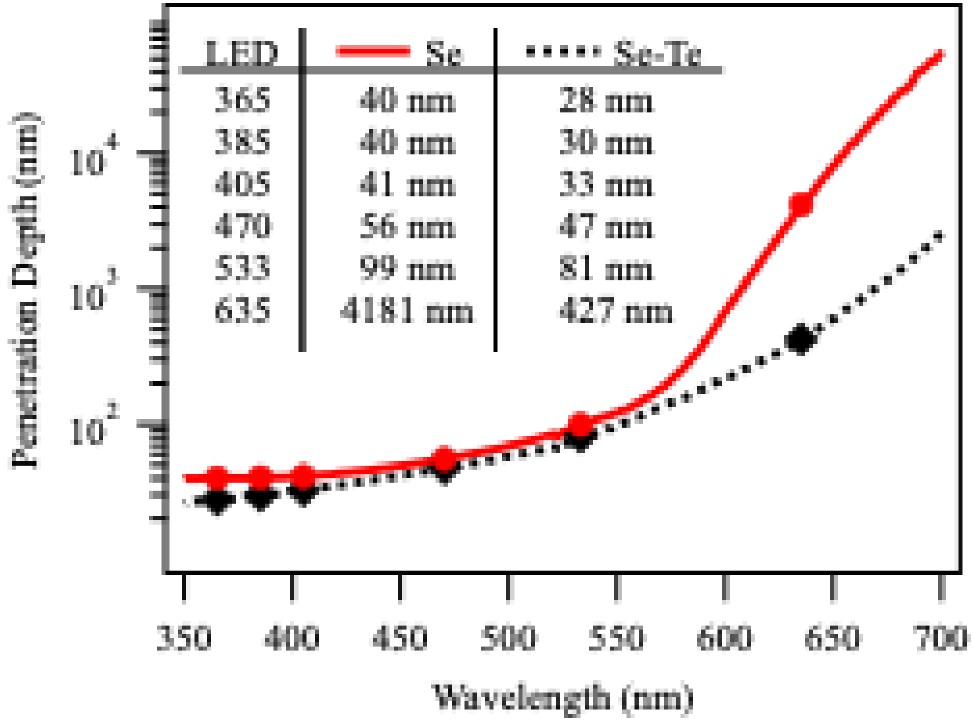
- Long wavelengths have low CE in a-Se
  - Short wavelengths absorbed in under 50 nm a-Se
- Se-Te has higher CE for long wavelengths

➢ Utilizing stacked layers, we can:
  - Improve sensitivity to long wavelengths with Se-Te
  - Preserve high transport for short wavelengths with a-Se

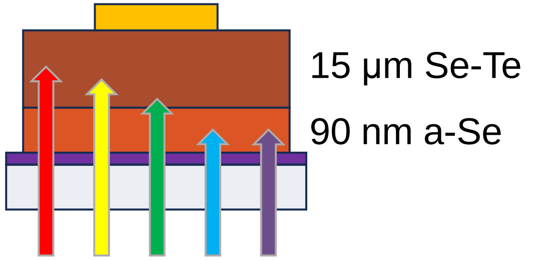
→ Goal: Investigate application of stacking in vertical (top) and lateral (bottom) devices

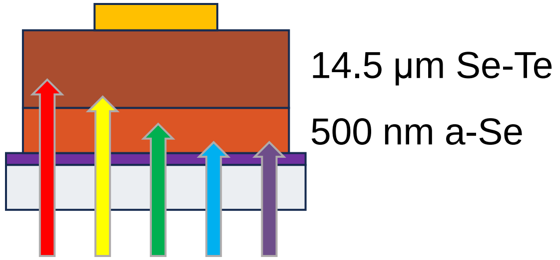
Stacked a-Se/Se-Te in Vertical Devices

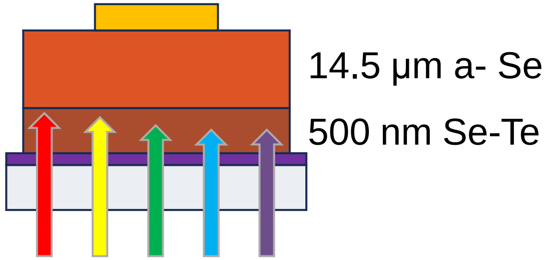
Penetration depth in Se and Se-Te



LED	Se	Se-Te
365	40 nm	28 nm
385	40 nm	30 nm
405	41 nm	33 nm
470	56 nm	47 nm
533	99 nm	81 nm
635	4181 nm	427 nm



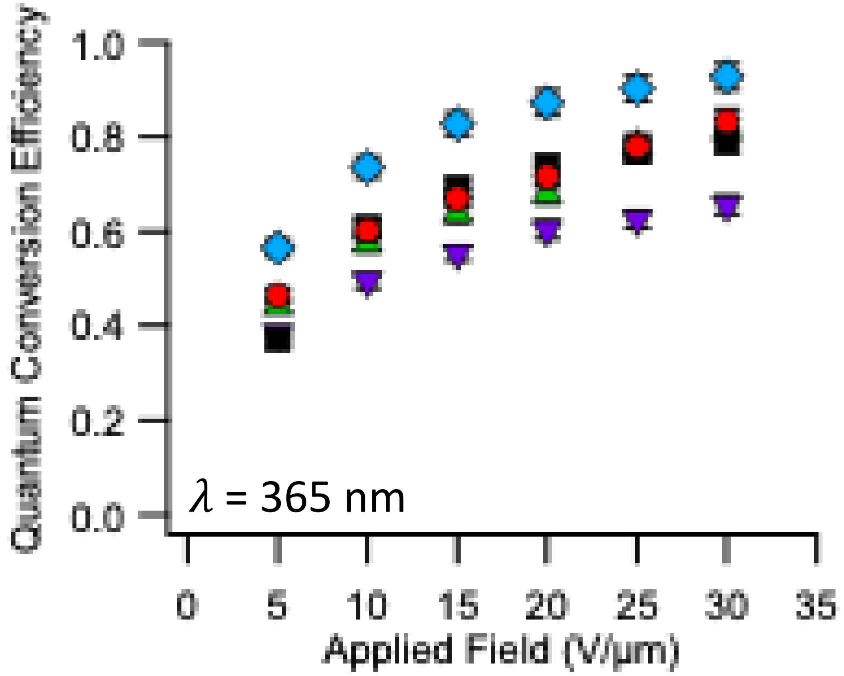




1. Vertical Stack with thin a-Se for short wavelengths, Se-Te for long wavelengths
2. Thick a-Se absorber layer, Se-Te transport layer
3. Thick Se-Te absorber layer, a-Se transport layer
4. Solid a-Se and Se-Te for control devices

Mirzanezhad et al., *ACS Opt. Mat*. (pending)

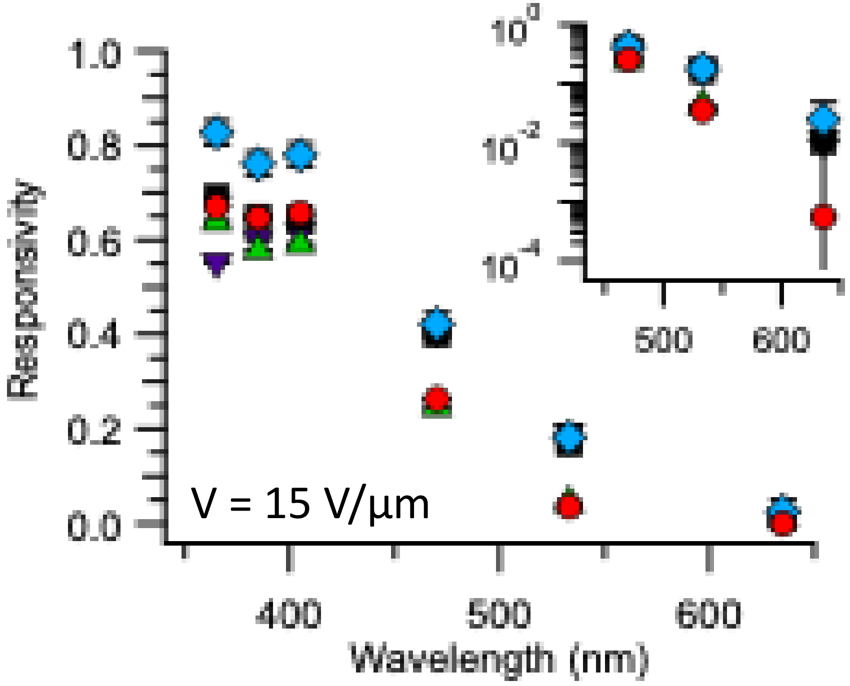
Vertical Structure: Improving QCE



- V1, V2, V4 perform similarly, in line with a-Se performance
- V5 – Se-Te absorption layer, Se transport layer – has lowest performance
- V3 – thin Se absorption, Se-Te long-wavelength – has highest CE

Mirzanezhad et al., *ACS Opt. Mat*. (pending)

Vertical Structure: Improving Sensitivity

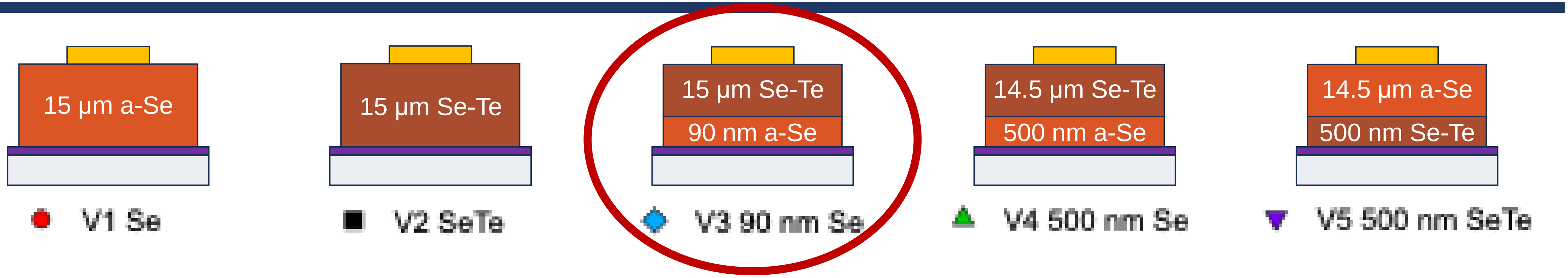


- V3 – thin a-Se with Se-Te for long wavelength – outperforms other samples
  - ~15% increase in CE at short wavelengths
  - Maintains sensitivity at long wavelengths

→ Allows for high CE at low fields

Mirzanezhad et al., *ACS Opt. Mat*. (pending)

Vertical Structure: Improving Sensitivity

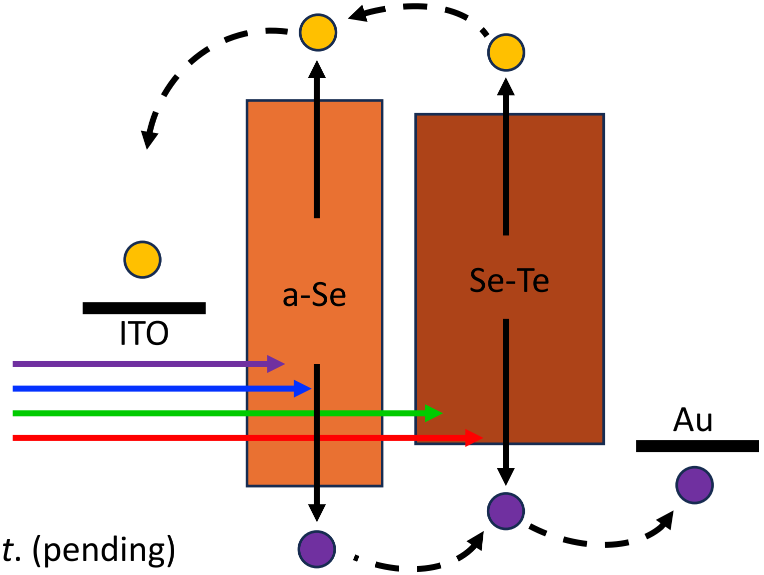


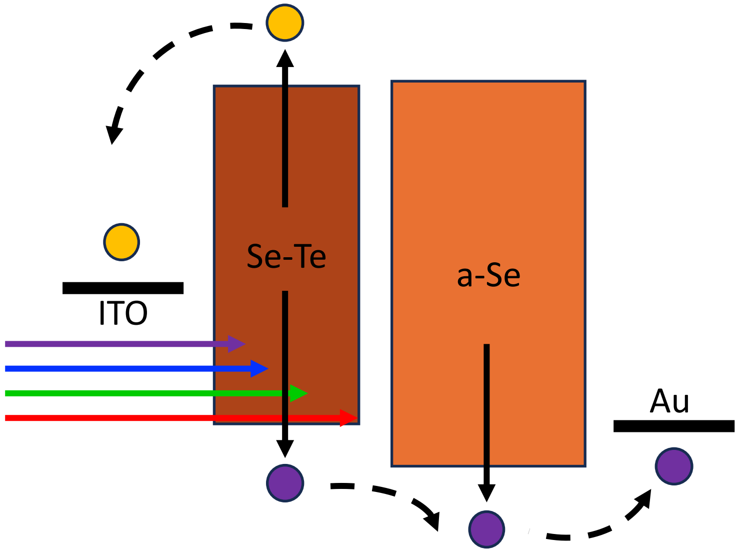
Stack with thin a-Se (90 nm) for absorbing short wavelengths and thick Se-Te (14.5 µm) for absorbing long wavelengths outperforms all others

Mirzanezhad et al., *ACS Opt. Mat*. (pending)

Vertical Structure: Improved Transport

- Transport occurs via trap-assisted hopping through shallow trap states
- Thin a-Se easily transports to Se-Te – thicker a-Se has more time to relax to shallow trap states, reducing extraction
- Se-Te as absorber layer has increased barrier for hole transport, with greater Schottky barrier from a-Se to Au → reduced extraction

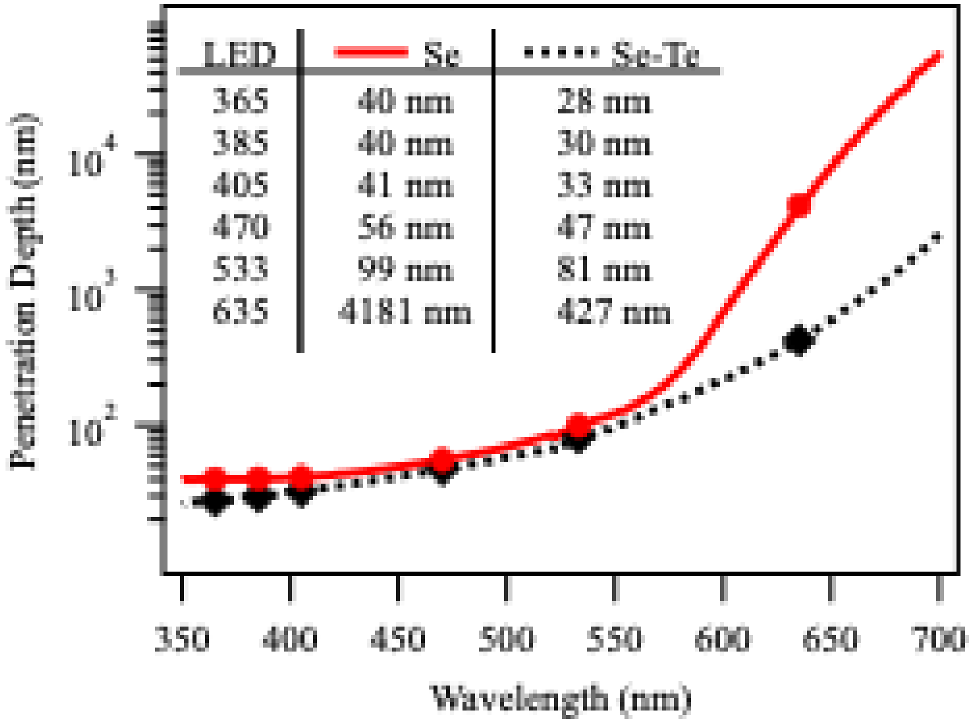




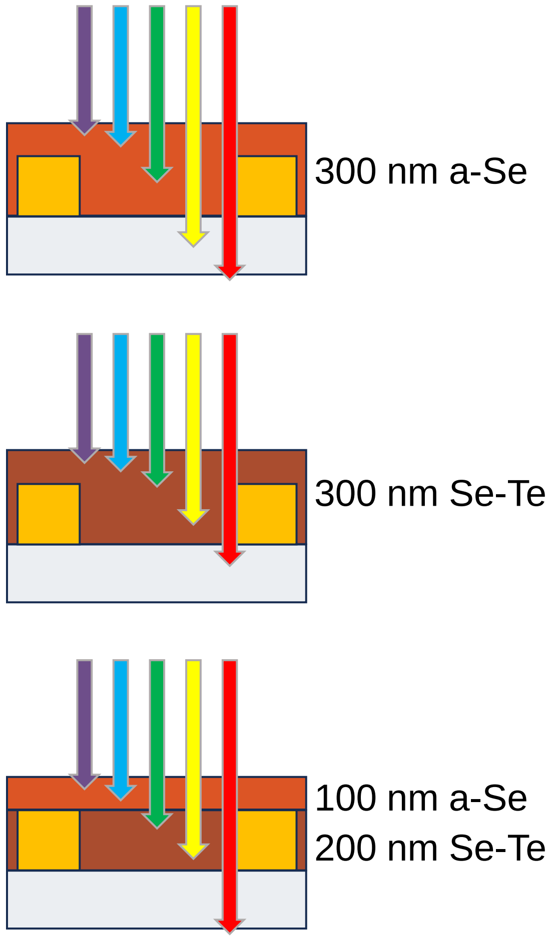
Mirzanezhad et al., *ACS Opt. Mat.* (pending)

Stacked a-Se/Se-Te in Lateral Devices

Penetration depth in Se and Se-Te



LED	Se	Se-Te
365	40 nm	28 nm
385	40 nm	30 nm
405	41 nm	33 nm
470	56 nm	47 nm
533	99 nm	81 nm
635	4181 nm	427 nm

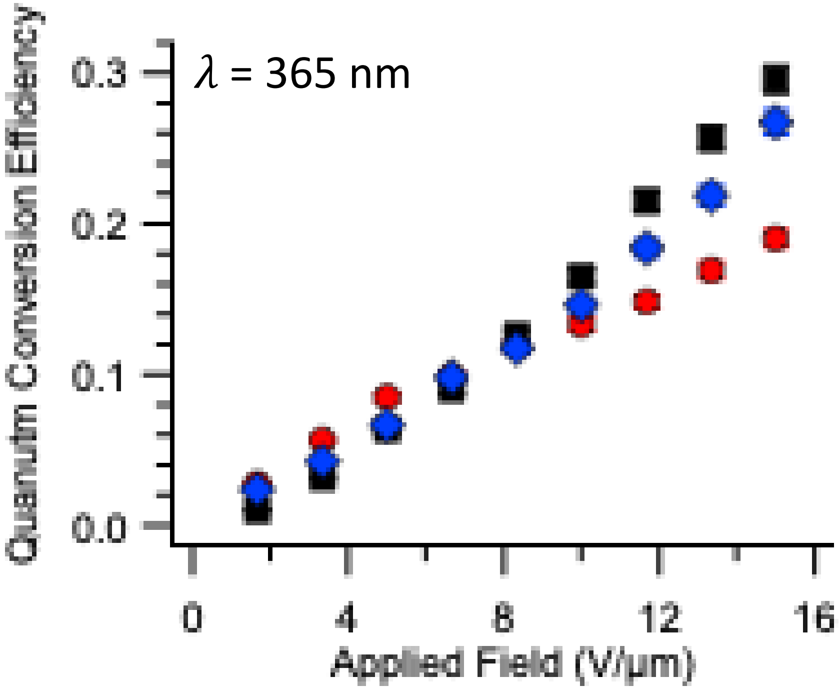


IDEs with 15 µm separation, 15 µm electrode width

1. Lateral a-Se, 300 nm
2. Lateral Se-Te, 300 nm
3. a-Se 100 nm top layer (short wavelength), Se-Te 200 nm bottom layer (long wavelength)

Mirzanezhad et al., *ACS Opt. Mat*. (pending)

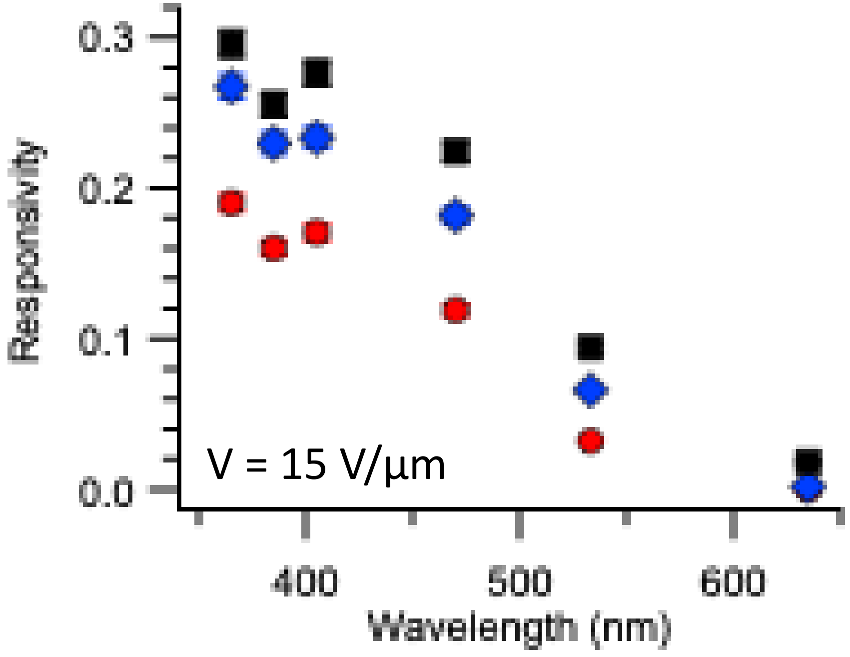
Lateral Structure: QCE



- All three have similar CE at lower fields
- As field increases:
  - Solid Se-Te becomes highest performer
  - Se underperforms compared to others (though in-line with literature)
  - Multilayer falls as a combination of the Se and Se-Te performance

Mirzanezhad et al., *ACS Opt. Mat*. (pending)

Lateral Structure: Responsivity



- Follows similar trends as 365 nm light:
  - Se-Te has highest performance, and improved long-wavelength sensitivity in line with penetration depth
  - a-Se underperforms in comparison
  - Multilayer has QCE better than equal combination of the two, but still falls short compared to solid Se-Te

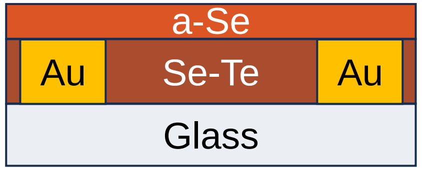
Mirzanezhad et al., *ACS Opt. Mat.* (pending)

Abbaszadeh et al., *IEEE Elec. Dev. Let.* (2011), v 32, 9, p 1263

Lateral Structure: Responsivity

● L1 Se

■ L2 Se-Te



◆ L3 Multilayer

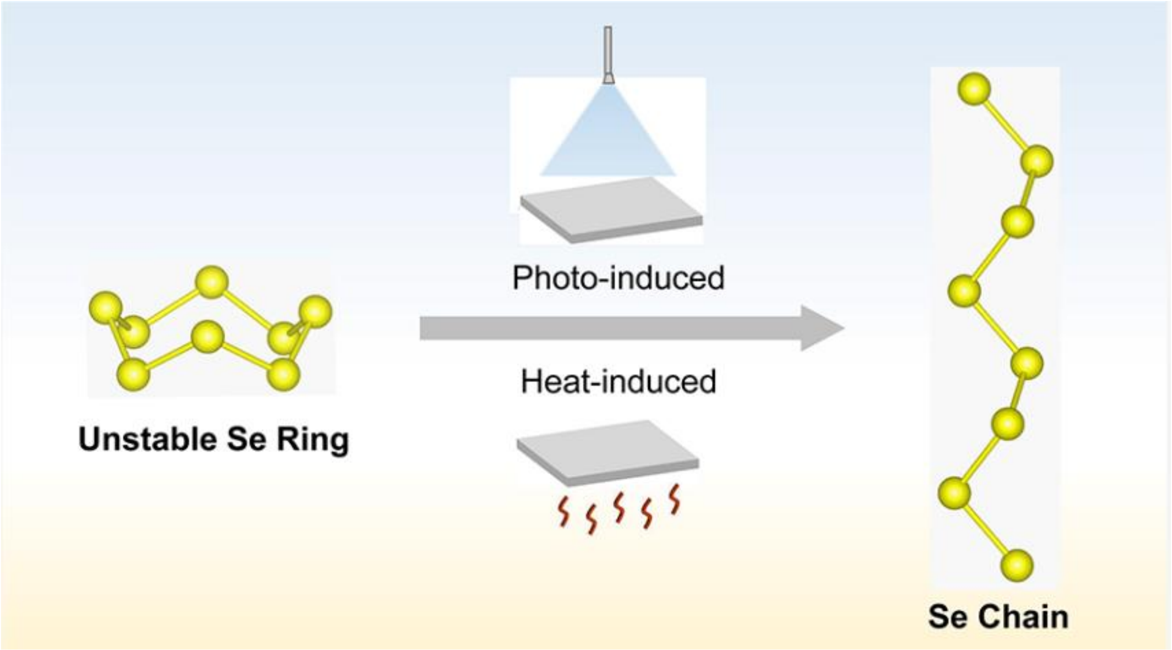
Solid Se-Te lateral device maintains the highest performance in CE and sensitivity.

Mirzanezhad et al., *ACS Opt. Mat*. (pending)

Lateral Structure: Transport

- a-Se forms in disordered "ring" structure
- Heat (used during fabrication) and light induce transformation to disordered chain structure

→ Transport across non-bonded atoms may be reduced, creating decreased CE for fields perpendicular to growth/chain direction



W. Lu *et al.*, "Structure of Amorphous Selenium: Small Ring, Big Controversy," *J. Am. Chem. Soc.* (2024), v 146, 9, p 6345

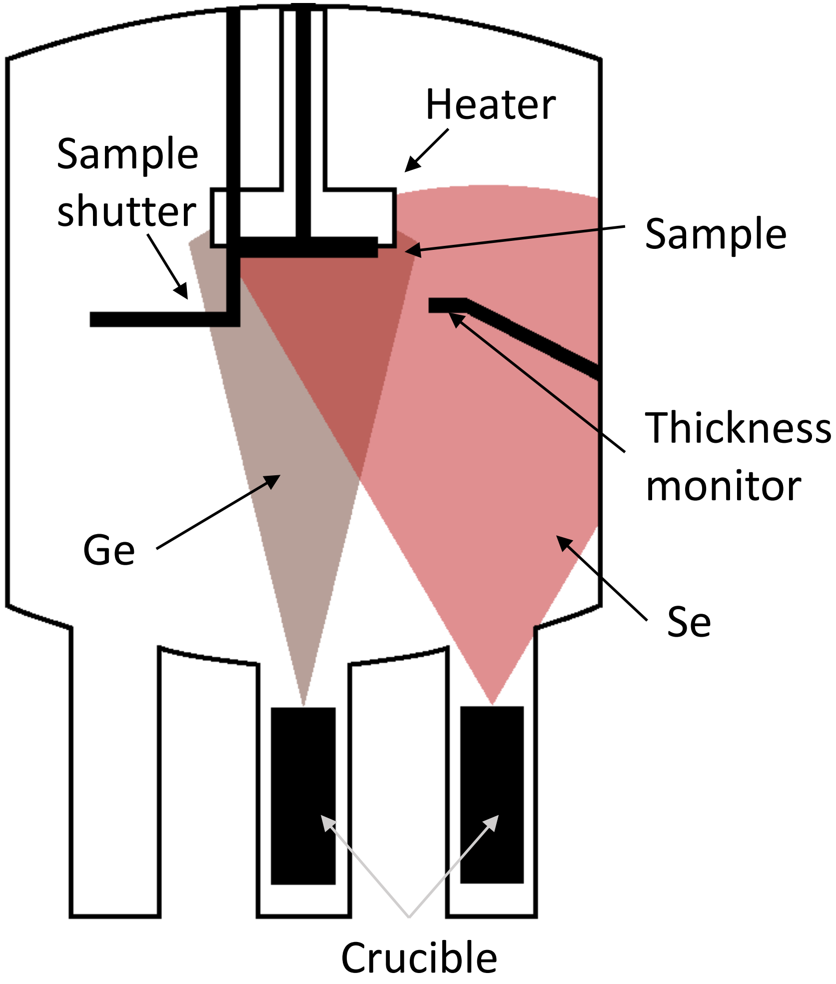
Mirzanezhad et al., *ACS Opt. Mat*. (pending)

Key Takeaways

- Alloying selenium (Se) with tellurium (Te) enhances long-wavelength sensitivity
- Adding Te reduces QE at low fields for short wavelength. High field recovers the reduced QE.
- Stacked configurations (a-Se and Se-Te) of vertical structure outperformed Se-Te devices.
- Uniform Se-Te configuration of lateral structure outperformed Stacked configurations.

Future Direction and Research Opportunities

- Expand experimental analysis of alloy compositions
  - Looking at evaluating the effect in impact ionization
  - Long-term stability
  - Photo-induced effect
- Develop co-deposition capabilities of Se and Ge to achieve high quality, uniform films
  - Controlling the electron mobility
  - Tuning optical and electronic properties



Radiological Instrumentation Laboratory (RIL)

Dr. Shiva Abbaszadeh
Electrical & Computer Engineering
sabbasza@ucsc.edu

Postdoctoral Scholars
- Dr. Kaitlin Hellier
- Dr. Jennifer Ott (SCIPP)

Graduate Students
- Gregory Romancheck (UIUC)
- Akyl Swaby
- Greyson Shoop
- Daniel Fiallo
- Kimia Gholemi
- Mohammadreza Mohseni Ferezghi
- Hamid Mirzanezhad
- Spencer Balliet
- Molly McGrath

Undergraduate Students
- Max Teichera
- Evelyn Cooper

UC SANTA CRUZ Baskin Engineering

Funding Provided by:

National Institute of Health
R01EB033466
NIH NIBIB

Department of Energy High Energy Physics
DE-SC0022343

Western Digital Corporation
WD

Pushing the limit of photodetection by bandgap engineering through alloying and stacking

---

Shiva Abbaszadeh

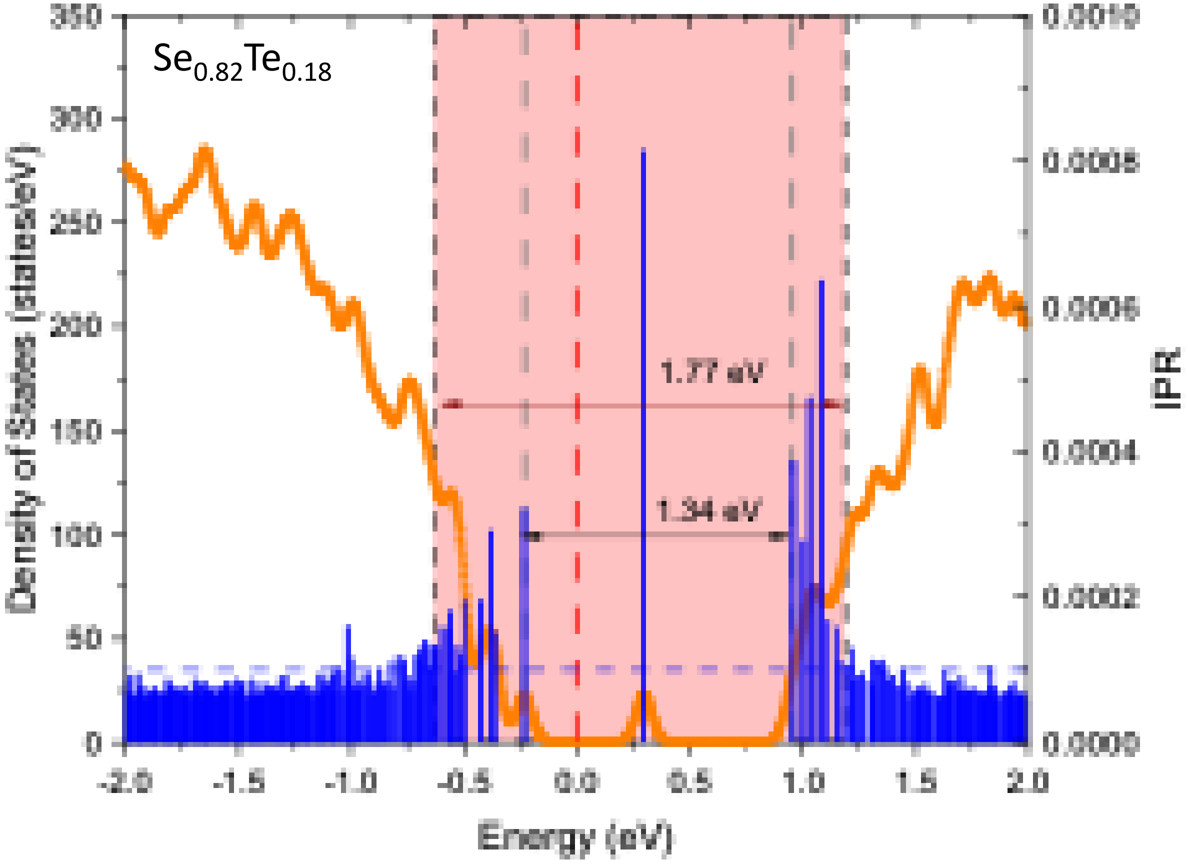
Radiological Instrumentation Laboratory

Electrical and Computer Engineering

ril.soe.ucsc.edu

UC SANTA CRUZ | Baskin Engineering

Modeling Density of States in Se-Te



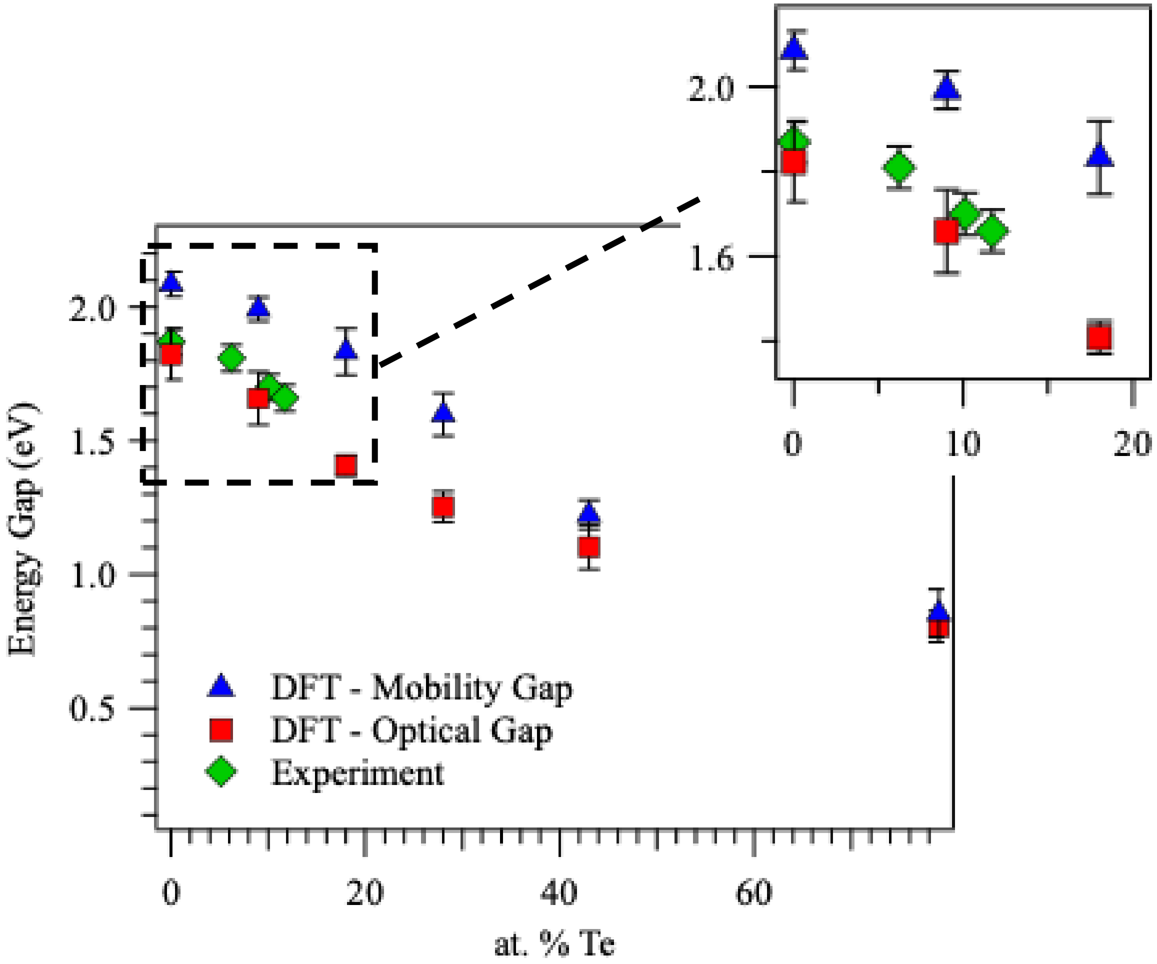
- Hybrid DFT using Vienna Ab initio Simulation Package (VASP), Perdew−Burke−Ernzerhof (PBE) exchange− correlation functional, disordered supercell with Stochastic quenching and structural relaxation
- DOS calculated for a-$Se_{1-x}Te_x$ (x=0, 0.9, 0.18, 0.28, 0.43, 0.79) → Optical & Mobility Gaps
- Inverse Participation Ratio (IPR) gives distinction between localized and delocalized states

Hellier et. al, *ACS AEM (*2023), v 5, 5, p 2678

Modeling Density of States in Se-Te

- Predicted mobility gap matches reported values for a-Se (2.0-2.2 eV)
- Predicted optical gaps in-line with those found in experiment
- Se-Te known to crystalize for Te>30% → reduced separation of mobility and optical gap

➢ Hybrid DFT allows for reasonable prediction of optical and electronic states in new materials



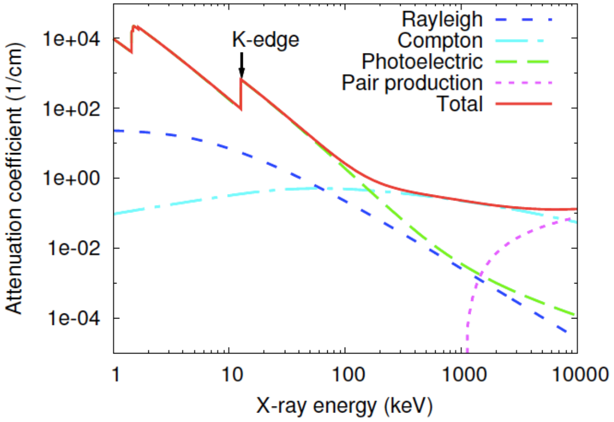
Hellier et. al, *ACS AEM (*2023), v 5, 5, p 2678

A-Se as Direct Conversion:
Pushing the Limit of Spatial Resolution

Commercial panel

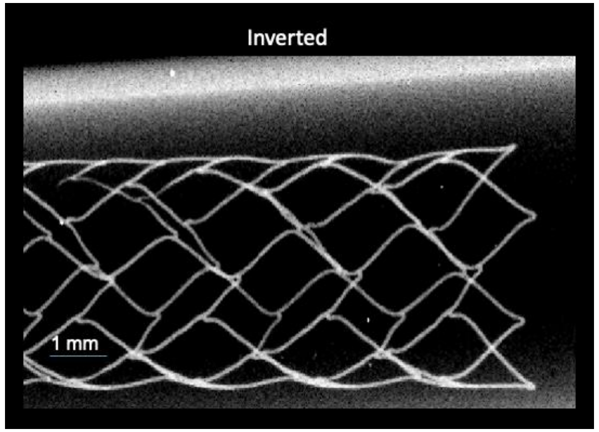
Anrad AXS-2430 a-Se mammography panel

Attenuation properties of a-Se



Specifications
3T active pixel sensor
300-400e RMS noise (improvements are possible)
25 µm pixel pitch
640 x 640 pixel array
1.6 x 1.6 cm active area

Aorta stent in glass vial, 25-50 µm wire diameter



Scott, Abbaszadeh et al., SPIE Medical Imaging, 2014.