An investigation of Arsenic doped $CdSe_xTe_{1-x}$ absorber layers for thin film photovoltaics using Density Functional Theory (DFT)

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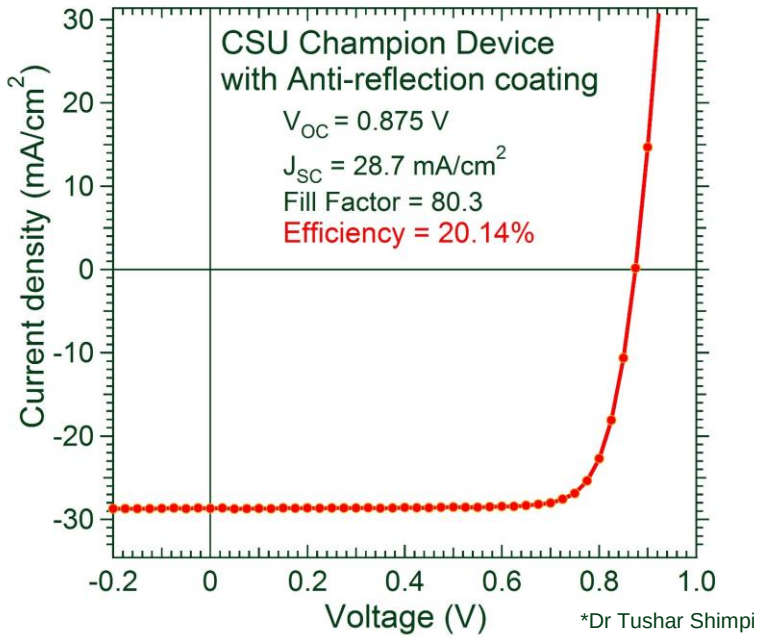
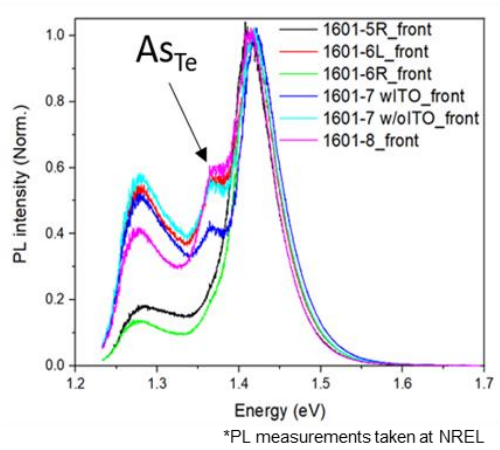
Next Generation PV Center

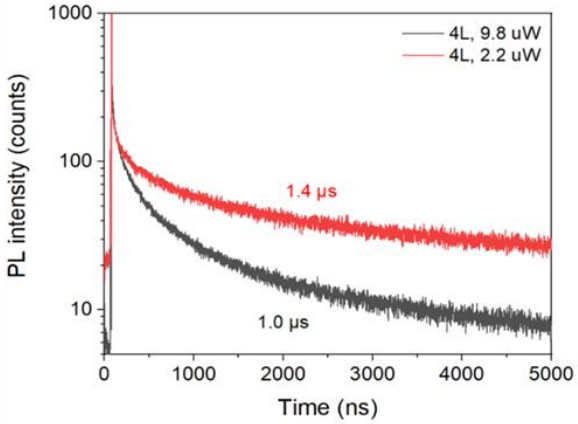
Motivation



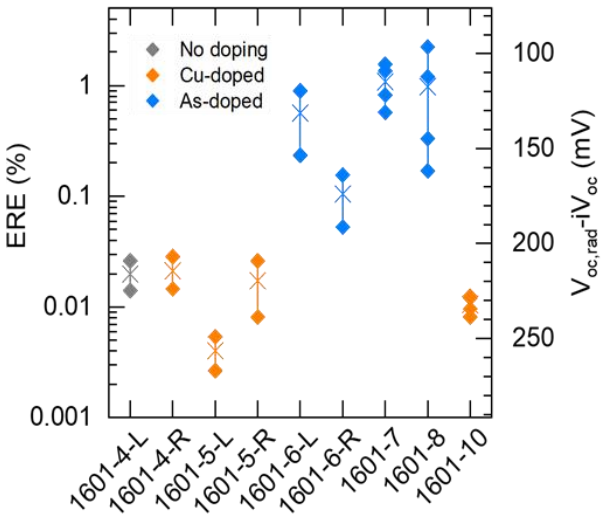
*Dr Tushar Shimpi



*PL measurements taken at NREL



*TRPL measurements taken at NREL



*ERE measurements taken at ASU

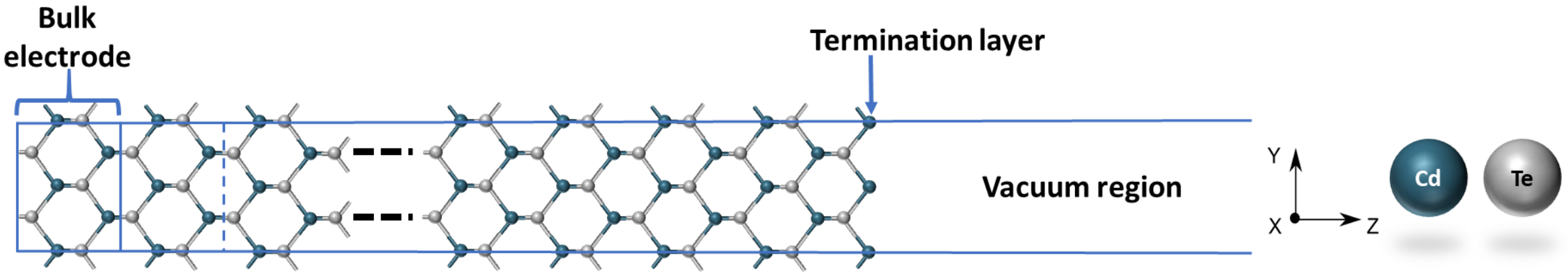
Champion device has CdSeTe/CdTe absorber layers

Arsenic doped CdSeTe/CdTe absorber layers have shown good lifetime and high External Radiative Efficiency

It is imperative to understand the properties of Arsenic doped CdSeTe/CdTe interface/surface to further improve device performance.

Atomistic simulation of interface

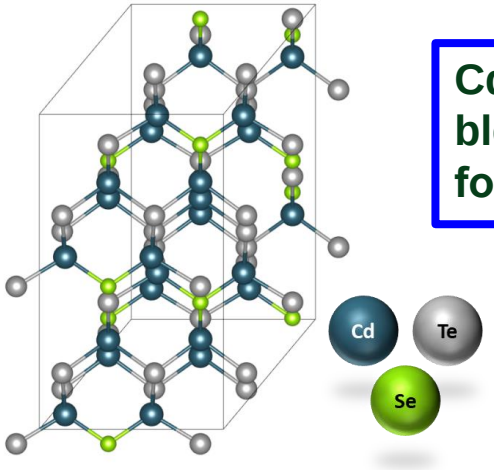
Quote	Interface is device- Nobel Laureate Herbert Kroemer
Interface modelling	Necessary to improve the device architecture
Current limitations	Band alignment simplification (does not include effects of strain or charge distribution), absence of defect states
Atomistic simulation	DFT enabled atomistic simulations provide detailed band diagram
QuantumATK, Synopsys	Suitable for 1 probe-surface (SGF**), 2 probe-interface simulations using NEGF method*; easy to use GUI



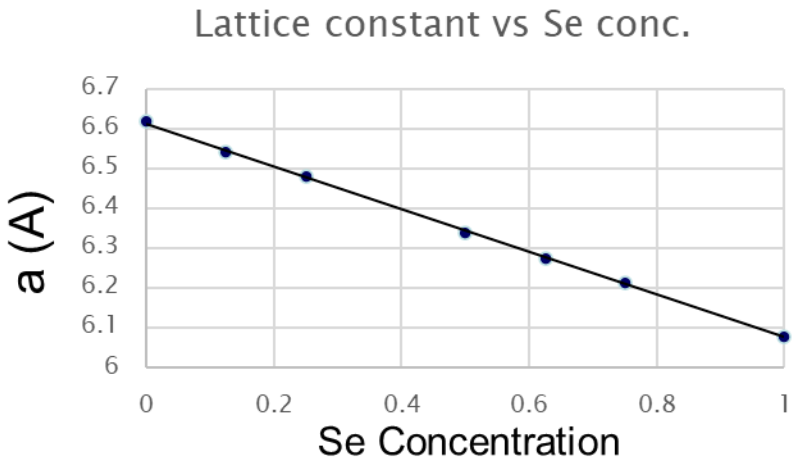
1 probe-surface model

*Non-equilibrium Green's Function
**Surface Green's Function

$CdSe_xTe_{1-x}$ model- Zinc blende



$CdSe_xTe_{1-x}$ Zinc blende structure follows Vegard's law.*



Se conc. (x)	a (A) this work	a (A) exp	a (A) theo
0	6.62	6.48[a], 6.47[a], 6.54[a]	6.62[a], 6.631[a], 6.54[a]
0.125	6.54	-	-
0.25	6.48	-	6.322[a]
0.5	6.339	-	6.407[a]
0.625	6.276	-	-
0.75	6.213	-	6.526[a]
1.0	6.08	6.084[a], 6.05[a]	6.207[a], 6.05[a]

Modeling Parameters:

- Exchange-Correlation functional: Local Density Approximation (LDA)
- Pseudopotential: FHI for Cd and Se, OpenMX for Te
- Linear Combination of Atomic Orbitals (LCAO) based basis sets: DoubleZetaPolarized for Cd and Se, Low basis set for Te.
- K-points:8x8x8
- Density mesh cutoff: 3000 eV
- Force Tolerance: 0.05 eV/A
- Stress Tolerance: 0.1 Gpa
- For a Se concentration x, values are reported for the lowest energy supercell configuration

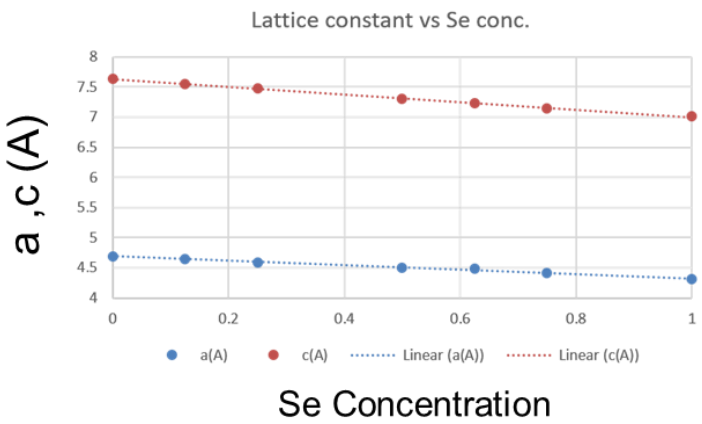
[a] Reshak et.al. Journal of Alloys and Compounds 509 (2011) 6737–6750

*Drew E. Swanson, James R. Sites, Walajabad S. Sampath Solar Energy Materials & Solar Cells 159(2017) 389–394

$CdSe_xTe_{1-x}$ model- Wurtzite

Se conc. (x)	a (A) this work	c (A) this work	a (A) exp	c (A) exp	a (A) theo	c (A) theo
0	4.69	7.64	4.57[a]	7.47[a]	4.68[a], 4.56[a]	7.65[a], 7.54[a]
0.125	4.64	7.55	-	-	-	-
0.25	4.59	7.47	-	-	4.563[a]	14.563[a]
0.5	4.496	7.3	-	-	4.437[a]	7.459[a]
0.625	4.48	7.227	-	-	-	-
0.75	4.405	7.15	-	-	4.429[a]	14.891[a]
1.0	4.311	7.008	4.3[a]	7.01[a]	4.34[a]	7.27[a]

$CdSe_xTe_{1-x}$ Wurtzite structure follows Vegard's law.**



Modeling Parameters:

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- **K-points:8x8x8**
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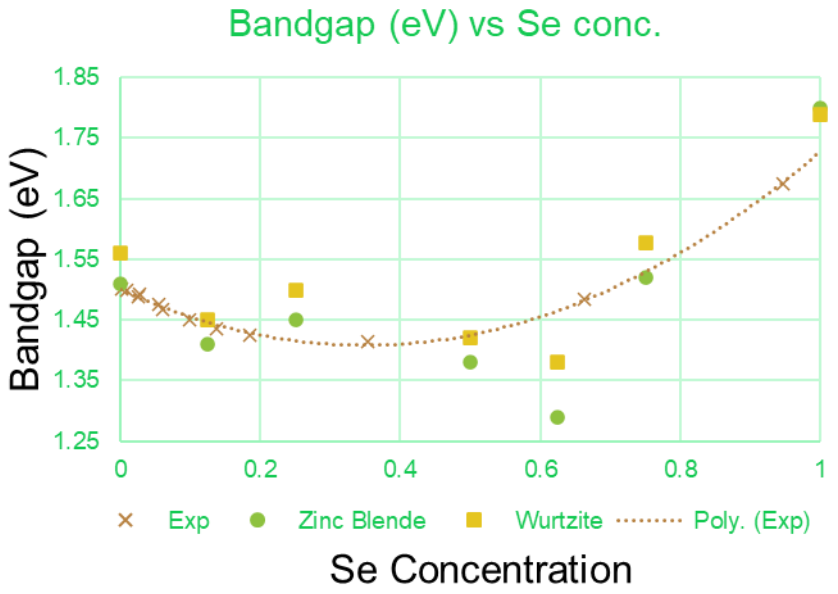
- **Stress Tolerance: 0.1 Gpa**
- **For a Se concentration x, values are reported for the lowest energy supercell configuration**

[a] Reshak et.al., Journal of Alloys and Compounds 509 (2011) 6737–6750

**N. Muthukumarasamy et. al., Sol.Energy 83 (2009) 522–526.

$CdSe_xTe_{1-x}$ model: Bandgap Study

Se conc. (x)	Crystal structure	E_g (eV) this work	E_g (eV) theo	E_g (eV) exp
0	Zinc blende	1.51	1.31[a], 1.51[b]	1.50*, 1.6[a], 1.4[a]
	Wurtzite	1.56	1.56[b]	
0.125	Zinc blende	1.41	1.46[b]	-
	Wurtzite	1.45	1.45[b]	
0.25	Zinc blende	1.45	1.44[a], 1.44[b]	-
	Wurtzite	1.50	1.49[b]	
0.5	Zinc blende	1.38	1.56[a], 1.43[b]	1.48[a]
	Wurtzite	1.42	1.42[b]	
0.625	Zinc blende	1.29	1.43[b]	-
	Wurtzite	1.381	1.37[b]	
0.75	Zinc blende	1.52	1.65[a], 1.45[b]	1.425[a]
	Wurtzite	1.578	1.55[a], 1.51[b]	
1.0	Zinc blende	1.80	1.76[a], 1.53[b]	1.82[a], 1.84[a]
	Wurtzite	1.79	1.60[a,b]	



Exp data taken from *Drew E. Swanson, James R. Sites, Walajabad S. Sampath, Solar Energy Materials & Solar Cells 159(2017) 389–394.

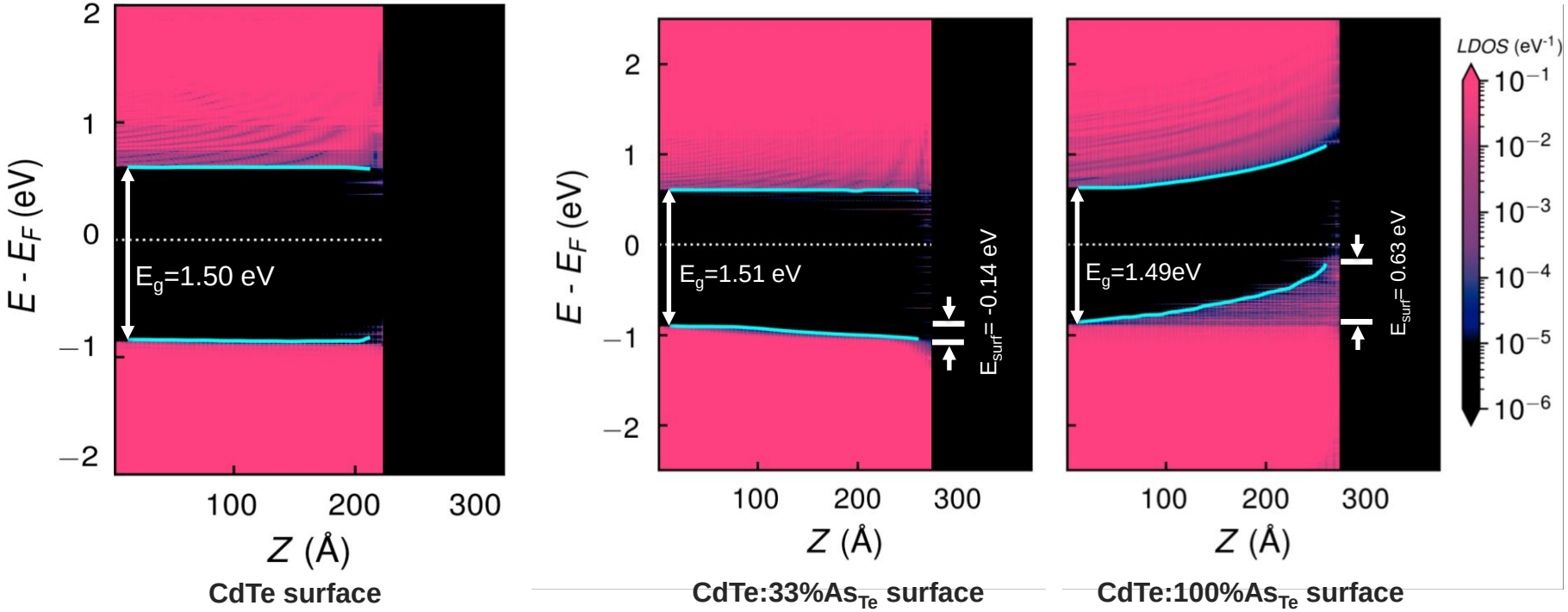
[b]Data from Dr. Pooja Goddard, Loughborough University.

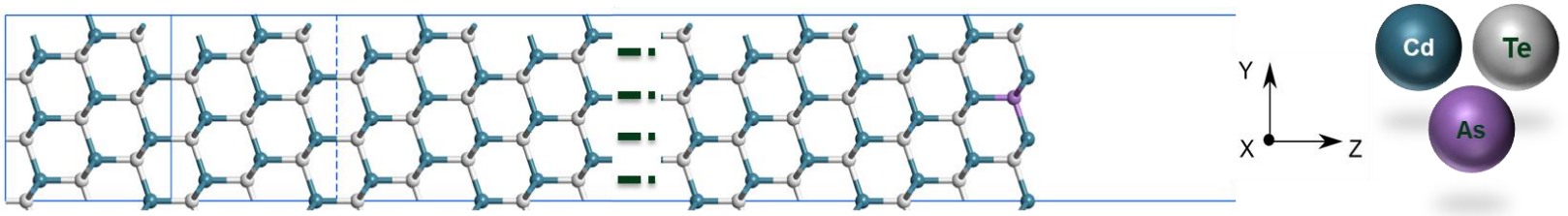
[a] Reshak et.al. Journal of Alloys and Compounds 509 (2011) 6737–6750

DFT-1/2 (LDA-1/2) correction scheme was used to calculate the bandgap.

The DFT LCAO model correctly predicts the lattice parameter, bandgap values and bandgap bowing of $CdSe_xTe_{1-x}$ alloy.

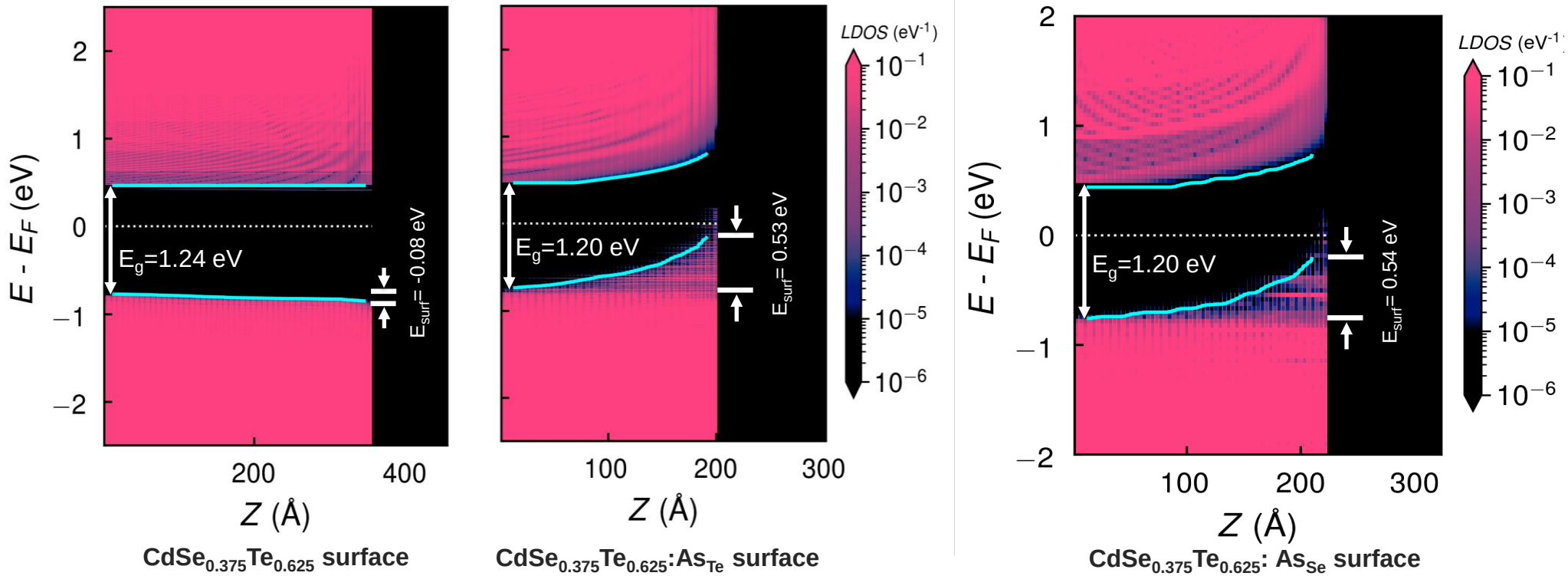
As_{Te} doped CdTe (111) surface

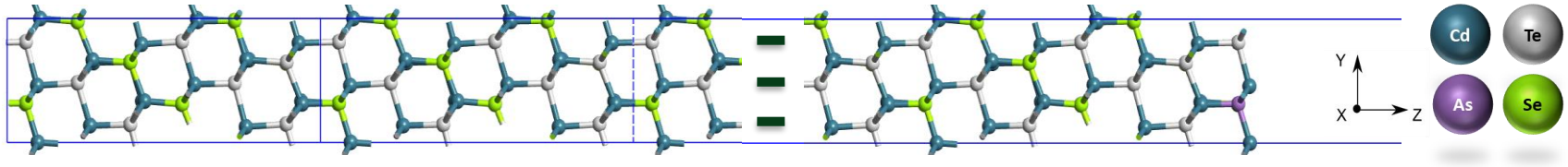




Monolayer As_{Te} doped CdTe surface gives favorable band alignment for hole transport

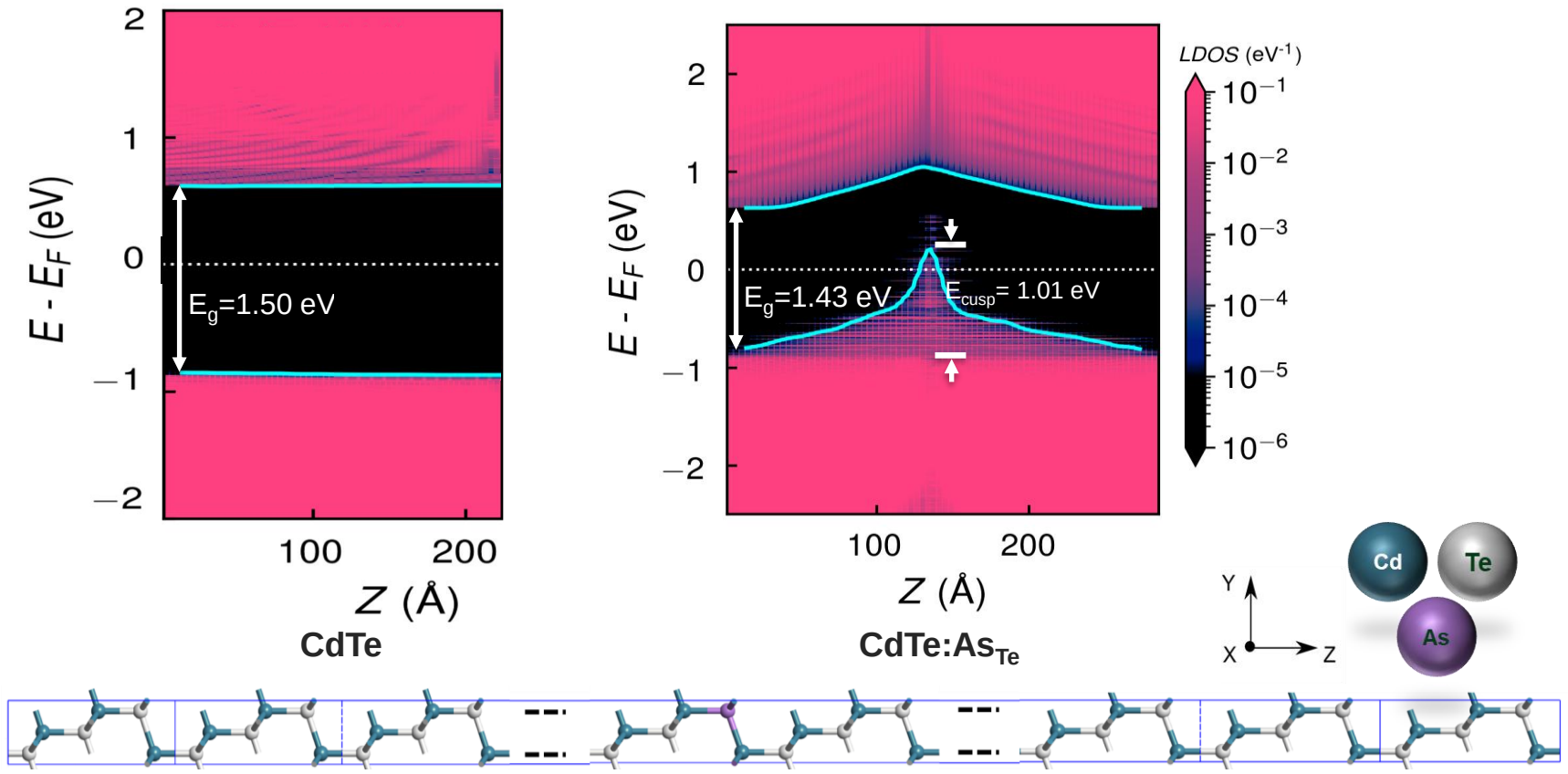
25% $As_{Te/Se}$ doped $CdSe_{0.375}Te_{0.625}$ (111) surface





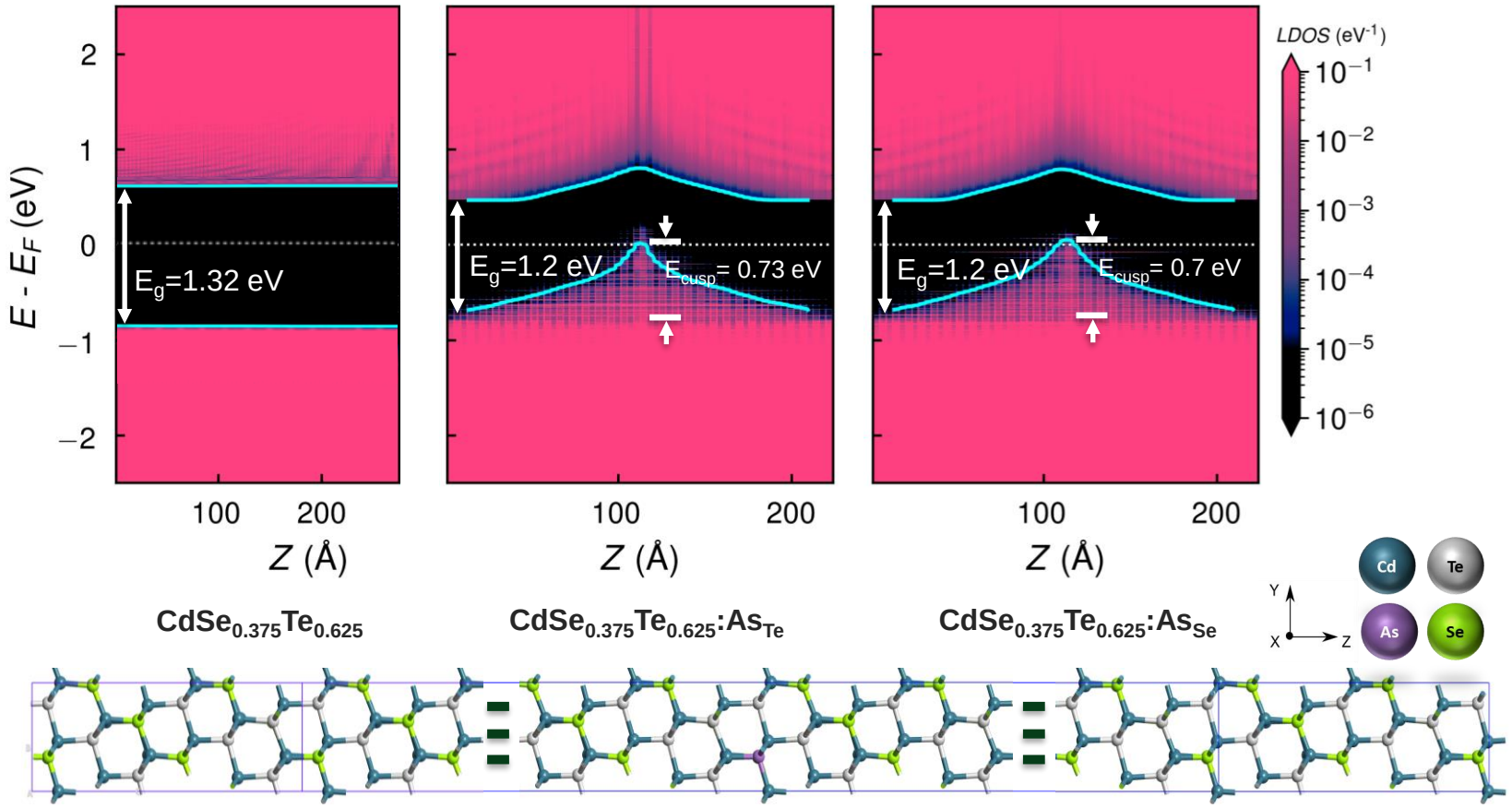
Favorable band alignment for hole transport with $As_{Te/Se}$ doped $CdSe_{0.375}Te_{0.625}$ surface could be achieved with lower doping concentration at surface

As_{Te} doped CdTe (111) film



- As_{Te} in bulk CdTe creates cusp in the Valence band with some interface states in the bandgap region.
- Conduction band bending up mitigates electron transport to the back of the device.

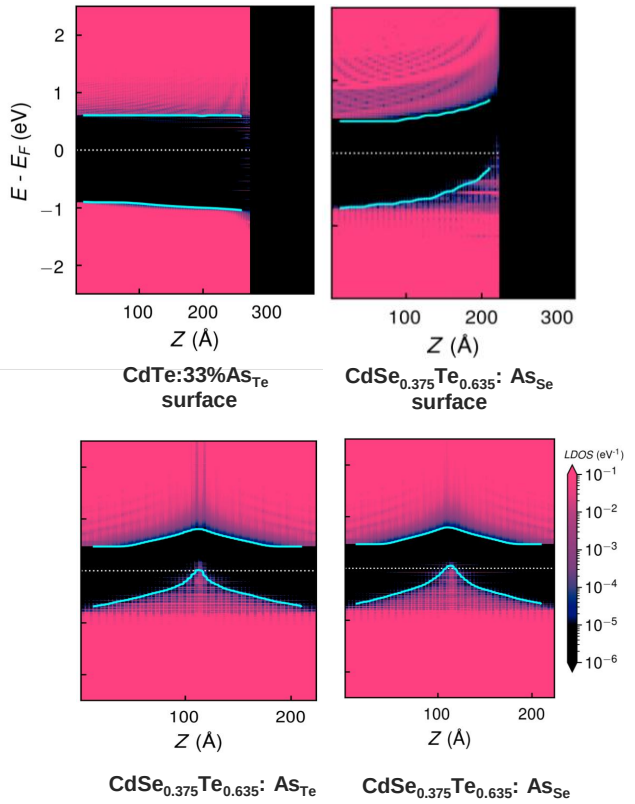
$As_{Te/Se}$ doped $CdSe_{0.375}Te_{0.625}$ (111) film



- $As_{Te/Se}$ in bulk $CdSe_{0.375}Te_{0.635}$ creates cusp in the Valence band with and a clean bandgap region.
- Conduction band bending up mitigates electron transport to the back of the device.

Conclusion

- Innovation – able to simulate As doped absorber materials using Density Functional Theory.
- The DFT LCAO model correctly predicts the lattice parameter, band gap values and bandgap bowing of $CdSe_xTe_{1-x}$ alloy.
- The CdTe surface model shows that band bending can be altered by changing the chemistry of the surface.
- The $CdSe_{0.375}Te_{0.625}$ surface model illustrates that favorable band bending for hole transport could be attained with lower concentration of $As_{Te/Se}$ at the surface.
- Arsenic doping of bulk $CdSe_{0.375}Te_{0.625}$ shows cleaner bandgap region than Arsenic doped bulk CdTe. The results indicate conduction band bending up which mitigates electron transport to the back of the device.



$CdTe:33\%As_{Te}$ surface

$CdSe_{0.375}Te_{0.635}$: As_{Se} surface

$CdSe_{0.375}Te_{0.635}$: As_{Te}

$CdSe_{0.375}Te_{0.635}$: As_{Se}

- Feasibility of modeling bulk Arsenic doped CdSeTe/CdTe absorber layer is shown. Work is in progress to simulate for Arsenic graded absorber model.

Acknowledgement

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Thank You for listening patiently!

Questions??