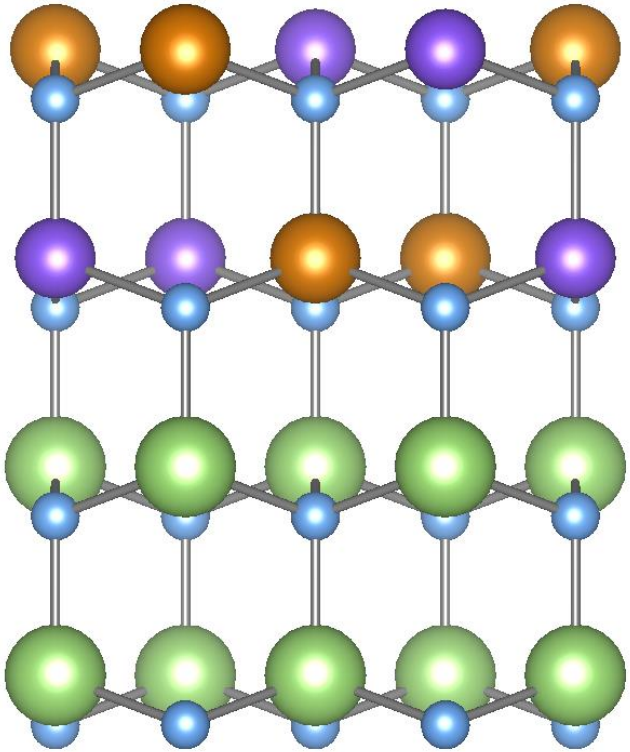
Zn-IV-nitrides for integration in electronic and photonic devices



Nicholas L. Adamski

Department of Electrical and Computer Engineering, University of California, Santa Barbara

Darshana Wickramaratne

United States Naval Research Laboratory

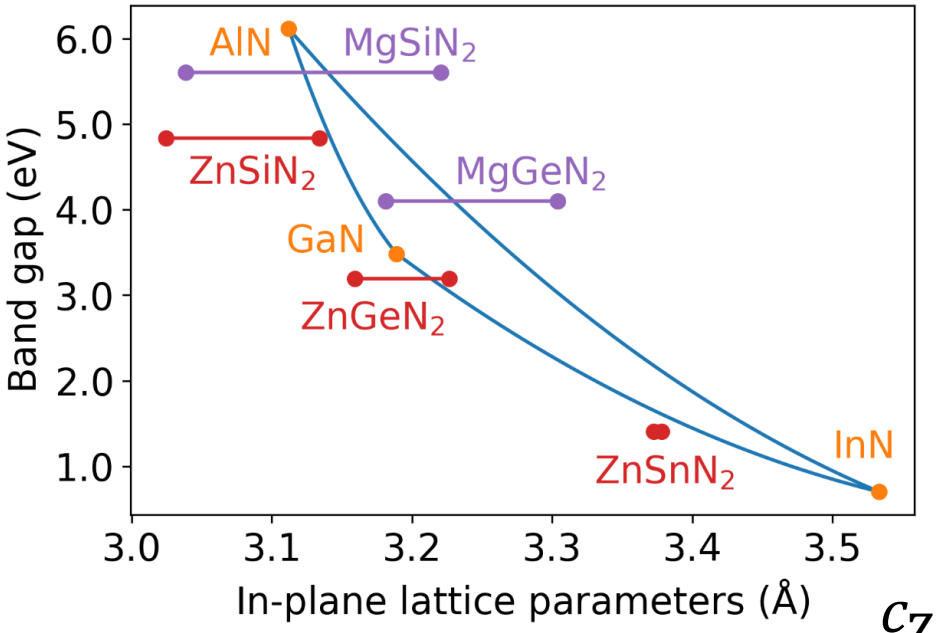
Chris G. Van de Walle

Materials Department,
University of California, Santa Barbara

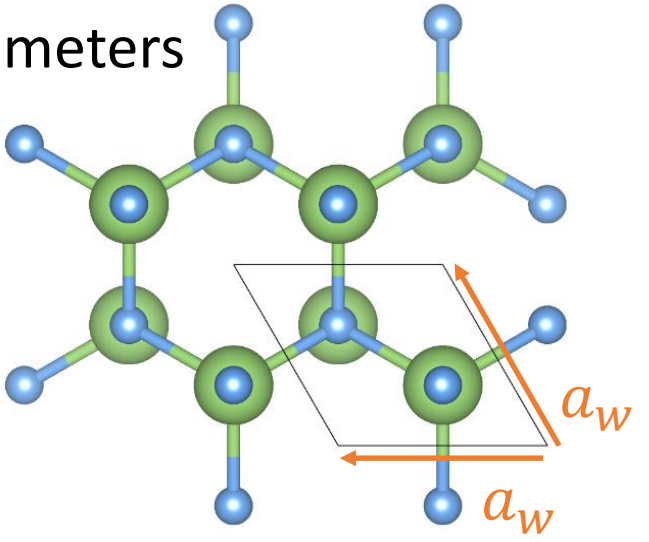
- This work was supported by the U.S. Army Research Office (ARO).

II-IV-Nitrides: Expanding the nitride design space

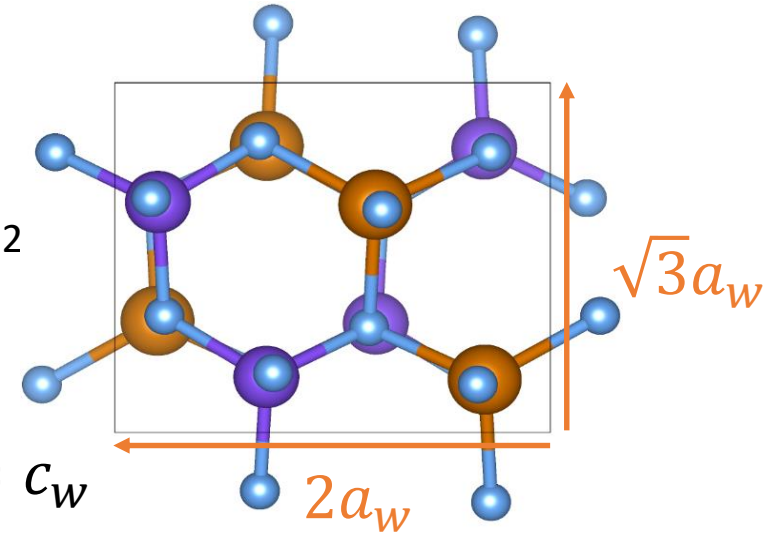
- Integrate II-IV-nitrides with III-nitrides
- Similar range of band gaps and lattice parameters
- Need information about
  - Band alignments
  - *n* and *p* type doping
  - Need polarization calculations



GaN



$ZnGeN_2$



$c_{ZnGeN_2} = c_w$

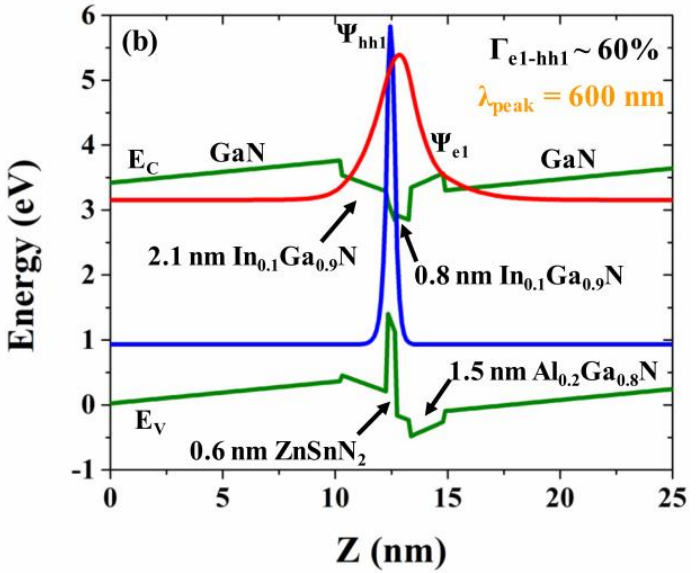
II-IV-Nitrides: Devices and applications

Can be grown high quality (MOCVD)

- M. R. Karim *et al*., Cryst. Growth Des. **19**, 4661 (2019)

Accurate knowledge of band offsets critical for optical devices

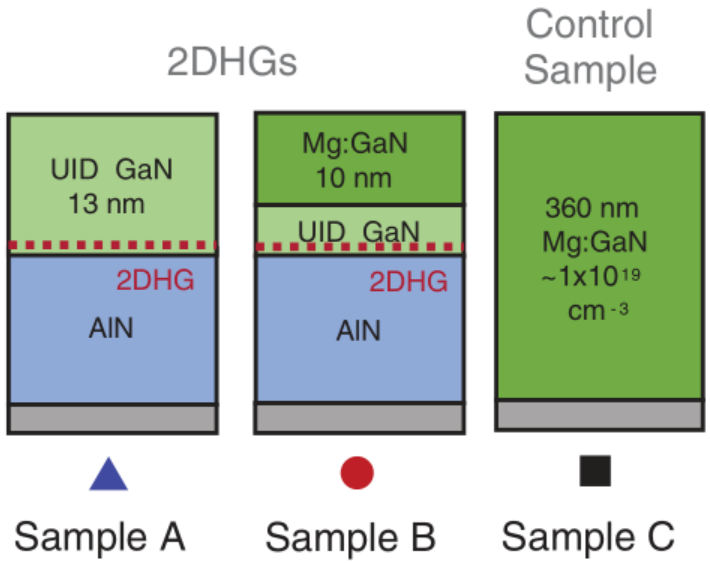
- Enhanced active region in quantum wells
  - ➢ Zn-IV-Nitride/InGaN emitters
- Barrier layers for UV emitters
- Solar absorbers over a range of band gaps



M. R. Karim *et al*., J. Appl. Phys. **124**, 034303 (2019).

Polarization properties at interfaces

- More options, more control
- 2DEGs and 2DHGs
  - ➢ Increased charges for power devices
- Zero-polarization interfaces
  - ➢ Reduced Stark effect for optical devices



R. Chaudhuri *et al*., Science **365**, 1454 (2019).

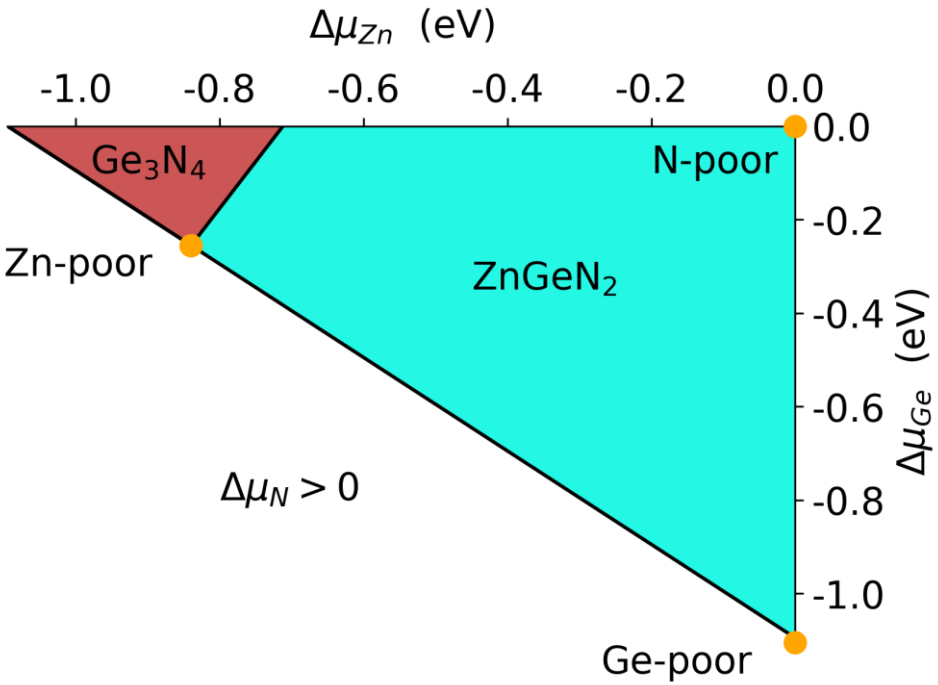
Point Defects: Formation Energy

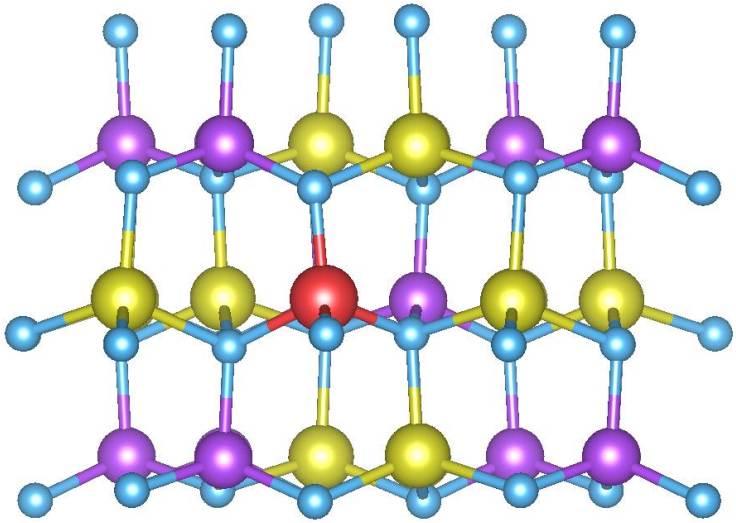
Density functional theory with the HSE hybrid functional.

J. Heyd *et al.*, J. Chem. Phys. **118**, 8207 (2003); ibid. **124**, 219906(E) (2006).

- Implementation in Vienna *Ab initio* Simulation Package.

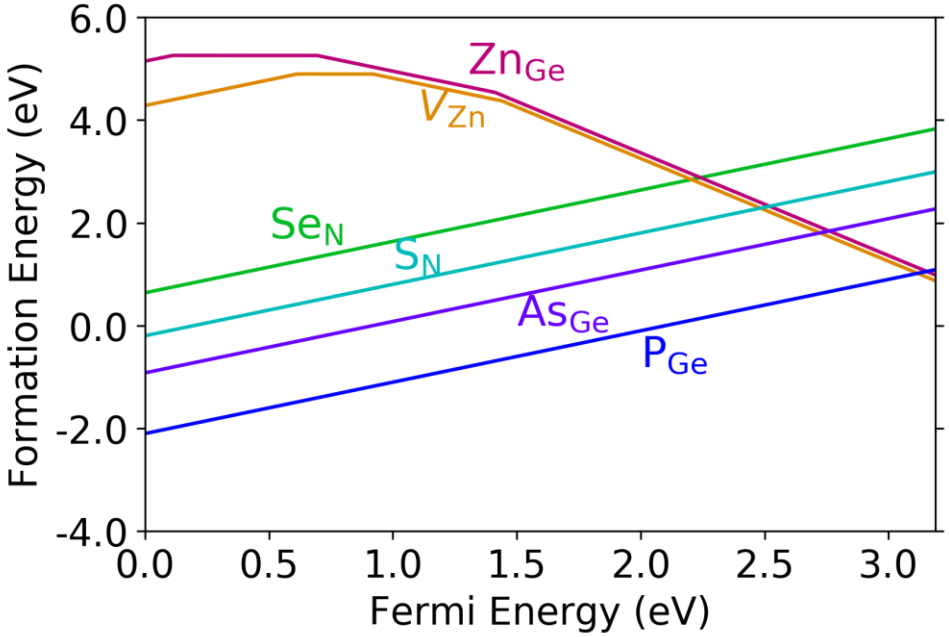
$$E_{form} = E_{defect} - E_{bulk} + \sum_i n_i \mu_i + n_e E_f$$

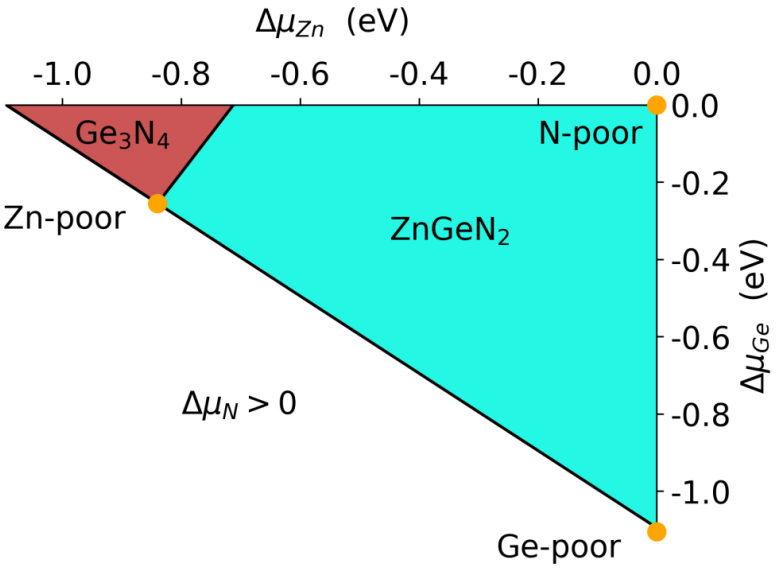


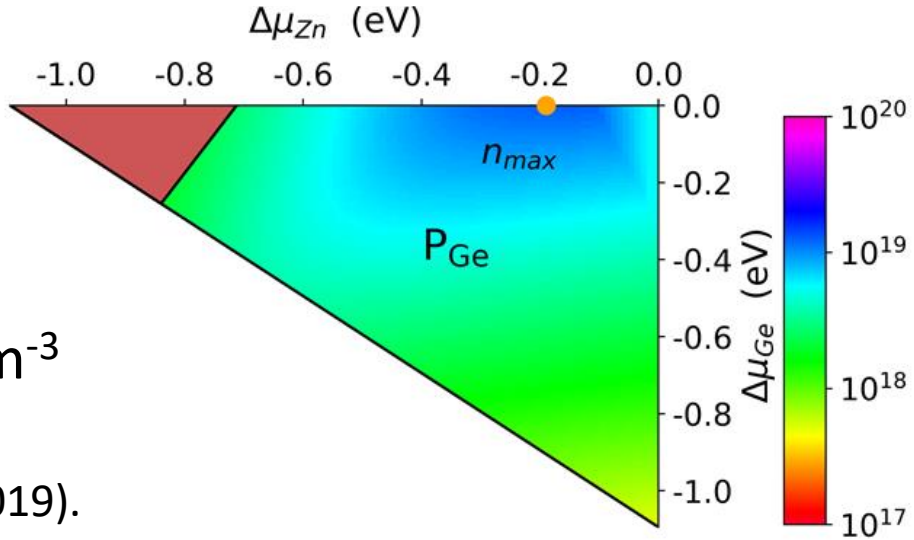


N. L. Adamski *et al.*, J. Appl. Phys. **122**, 195701 (2017).

$ZnGeN_2$: Donors



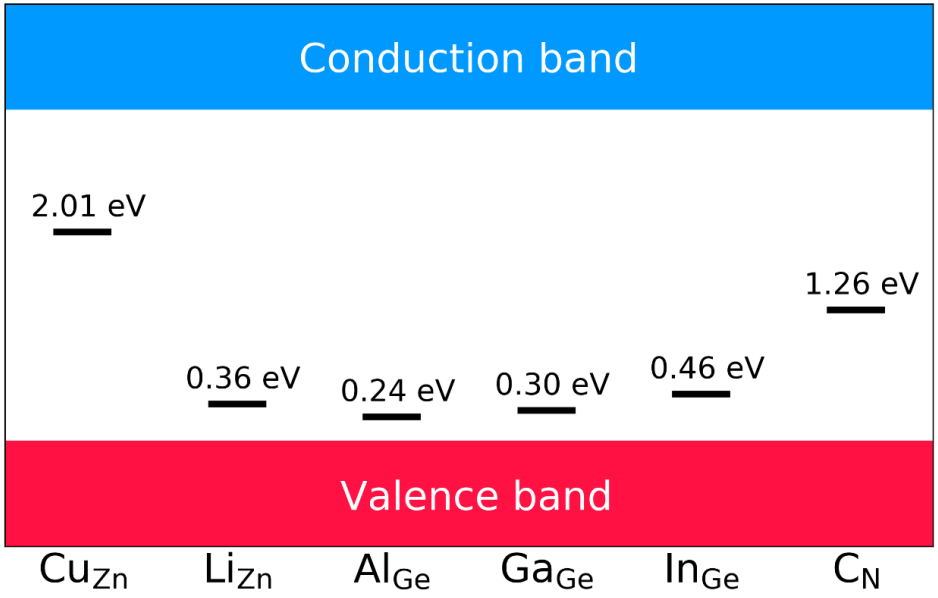


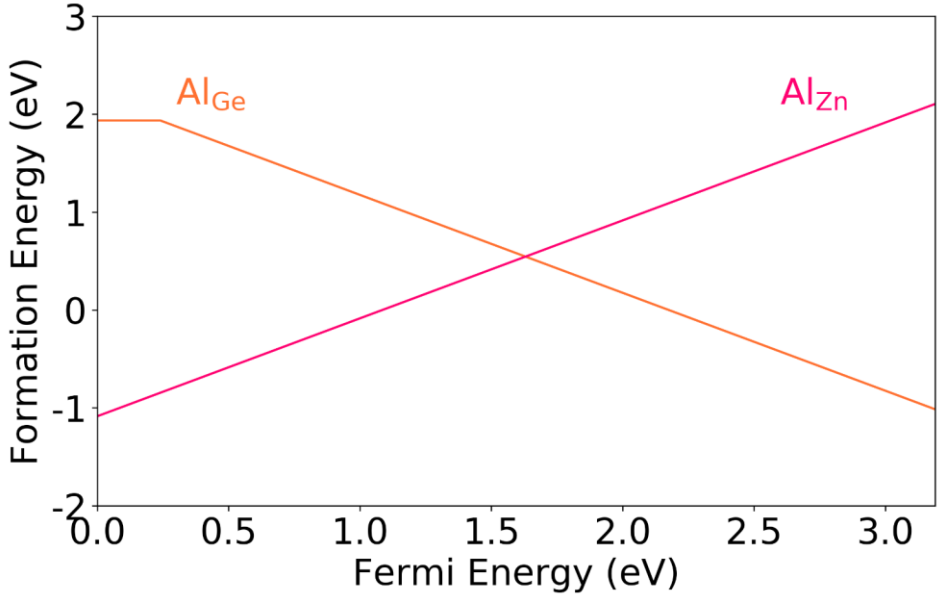


- P_{Ge} is the most stable donor
- Concentrations up to 1.3 x 10^{19} cm^{-3}

N. L. Adamski *et al.*, Phys. Rev. B **100**, 155206 (2019).

$ZnGeN_2$: Acceptors

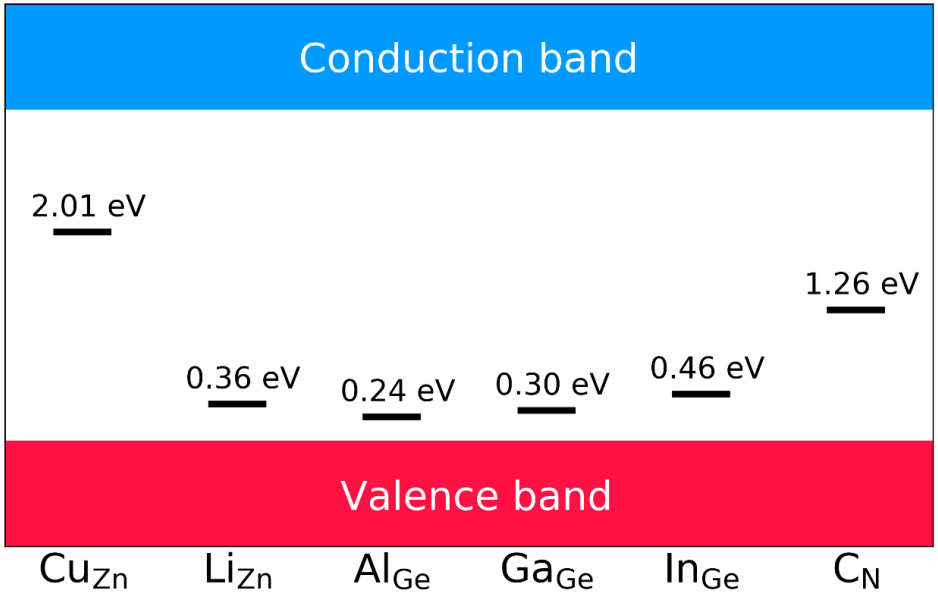


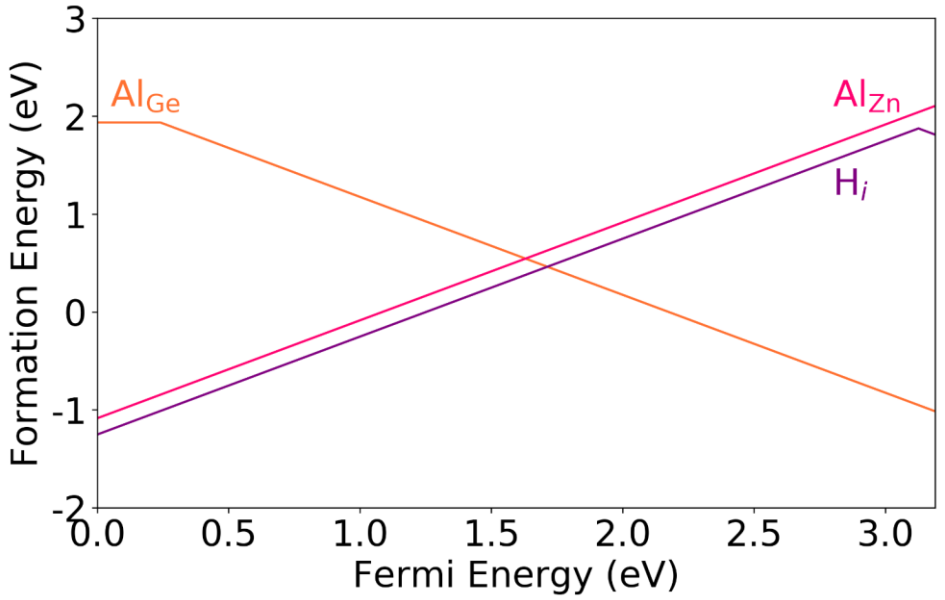


- Al_{Zn} is a shallow donor and will compensate Al_{Ge} acceptors.
- Charge balance will require equal concentrations.
- Fermi level pinned near mid gap.

N. L. Adamski *et al.*, Appl. Phys. Lett. **114**, 032101 (2019).

$ZnGeN_2$: Acceptors

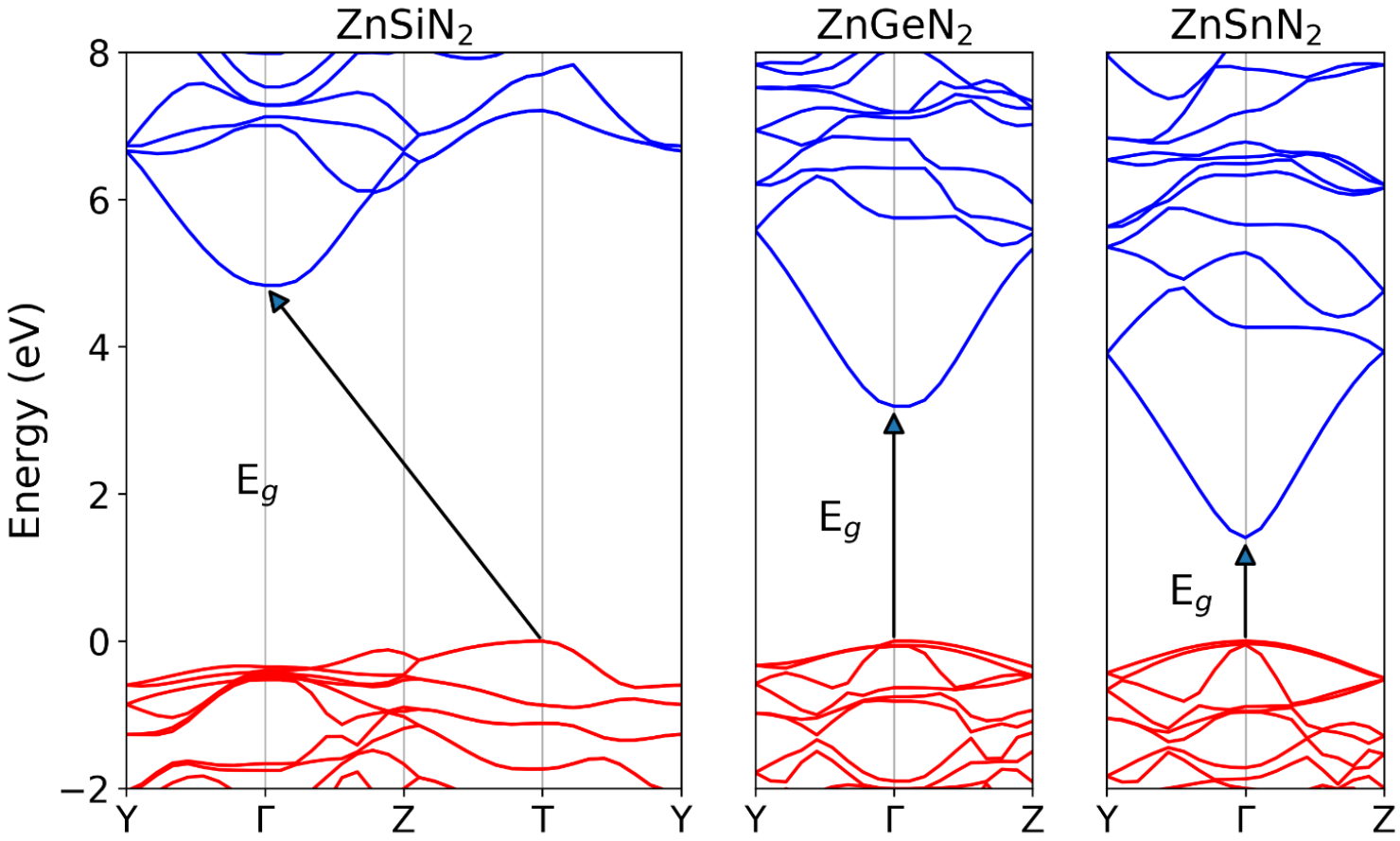




- Al_{Zn} is a shallow donor and will compensate Al_{Ge} acceptors.
- Charge balance will require equal concentrations.
- Fermi level pinned near mid gap.
- H_i will reduce Al_{Ge} formation energy.
- H suppresses Al_{Zn} formation.
- Possible to remove H post growth.

N. L. Adamski *et al.*, Appl. Phys. Lett. **114**, 032101 (2019).

Zn-IV-Nitrides: Band structure

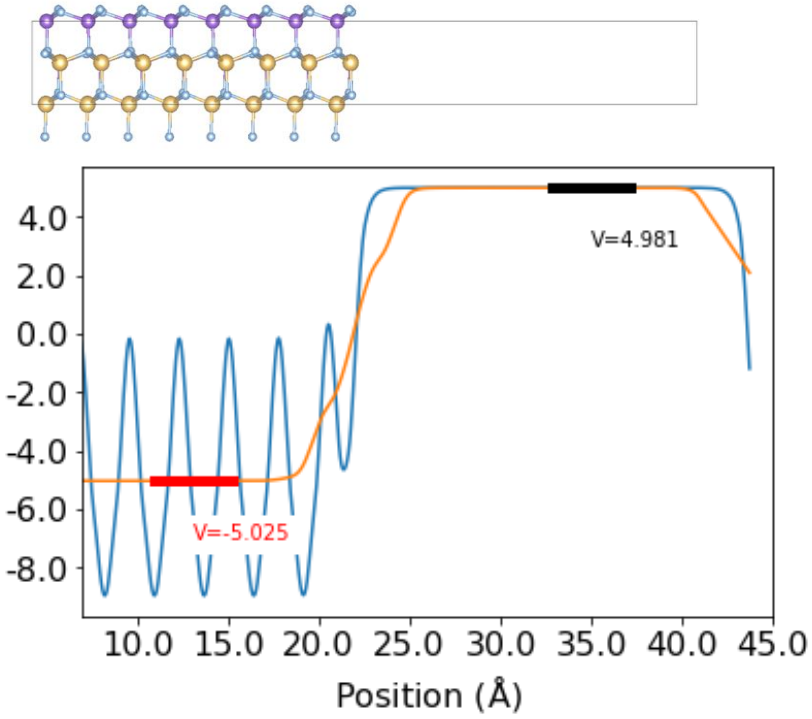


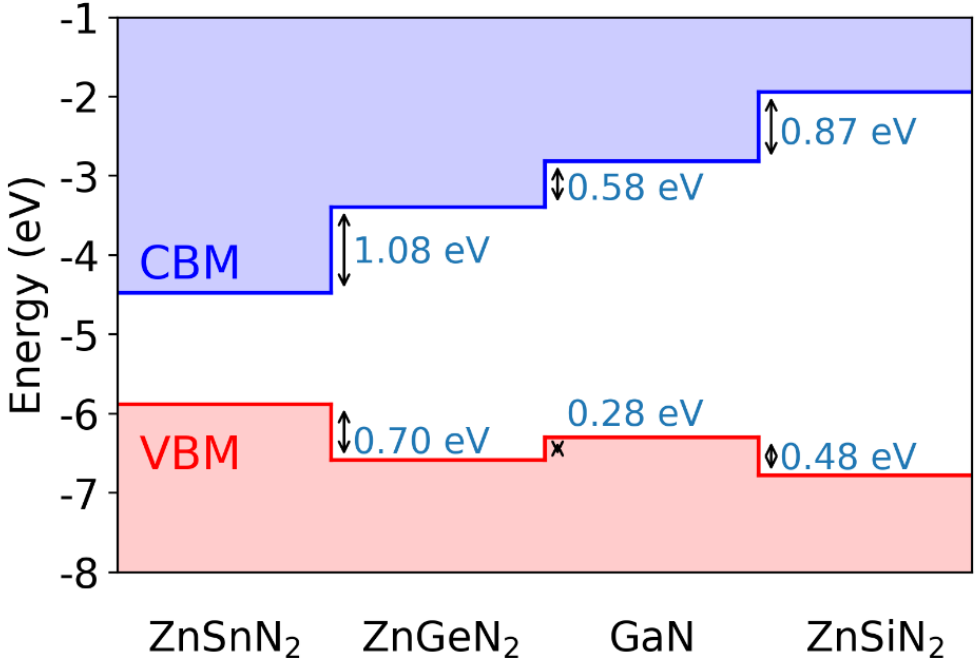
	$ZnSiN_2$	$ZnGeN_2$	$ZnSnN_2$
E_g (eV)	indirect: 4.83, direct: 5.18	3.19	1.40

Zn-IV-Nitrides: Band alignments

- Align the electrostatic potential to the vacuum energy level using calculations on slabs
- ➢ Determine band alignments

$ZnGeN_2$ [100] surface (m-plane)



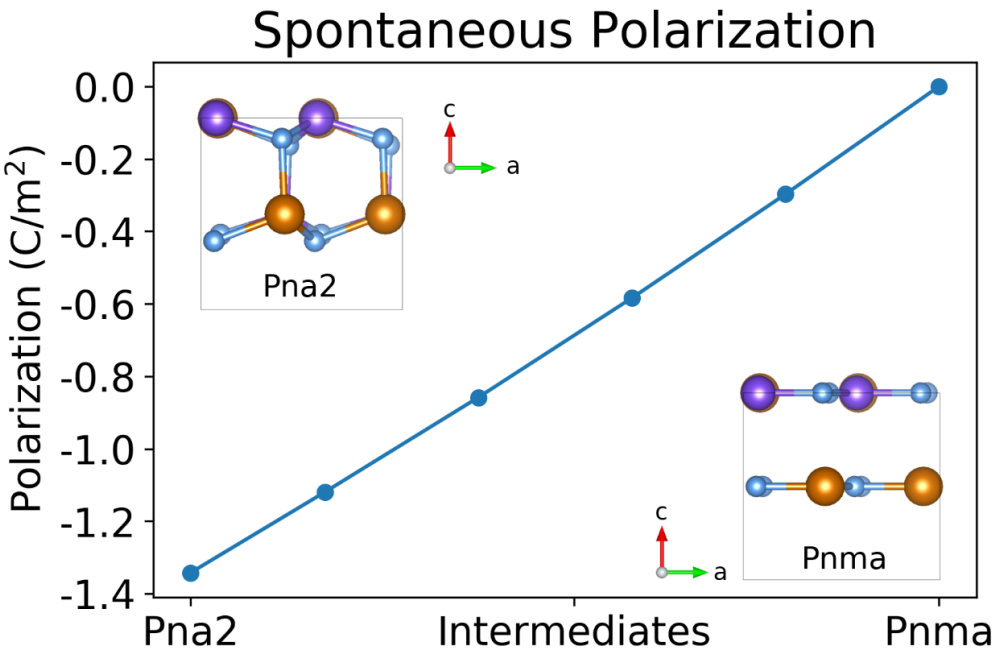


- CBM of $ZnGeN_2$ is 0.6 eV below that of GaN
- Staggered gap

$ZnSnN_2$ alignment in agreement with T. Wang *et al.*, Phys. Rev. B **95**, 205205 (2017).

Zn-IV-Nitrides: Polarization

- Polarization calculated with the modern theory of polarization
  R. D. King-Smith and D. Vanderbilt, Phys. Rev. B **47**, 1651 (1993)
- Measured referenced to layered, centrosymmetric structure

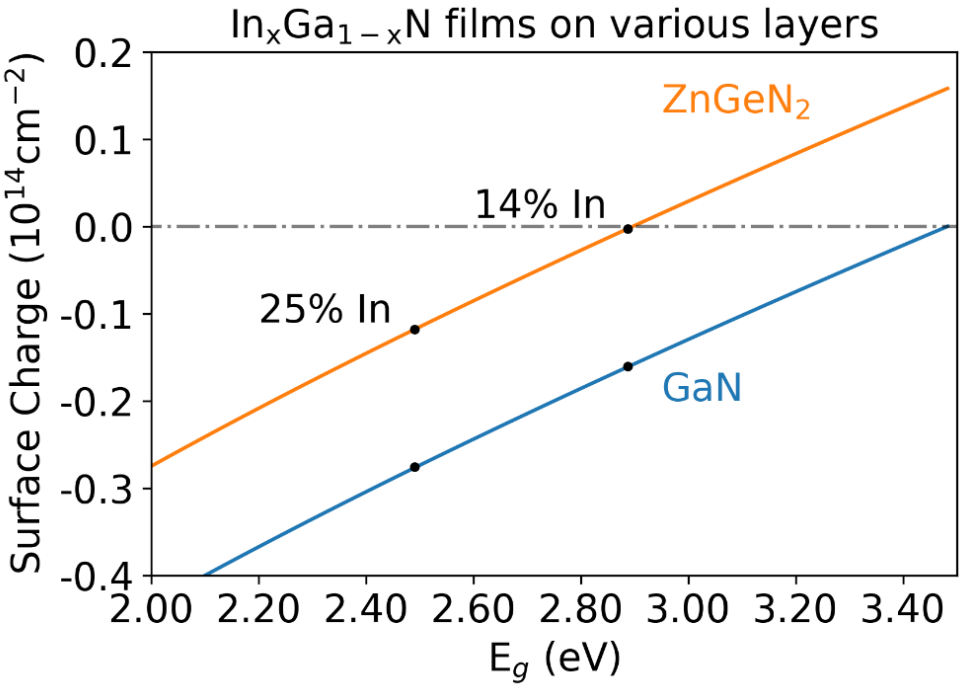


	$ZnSiN_2$	$ZnGeN_2$	$ZnSnN_2$	AlN	GaN	InN
$P_{SP,3}$	1.433	1.333	1.184	1.351	1.312	1.026

C. Dreyer *et al.*, Phys. Rev. X **6**, 021038 (2016).

Bound charges at strained interfaces

$$\sigma_b = (P_{SP}^m - P_{SP}^n) - \epsilon_1 \left(e_{31}^n - e_{33} \frac{C_{13}^n}{C_{33}} \right) - \epsilon_2 \left(e_{32}^n - e_{33} \frac{C_{23}^n}{C_{33}} \right)$$

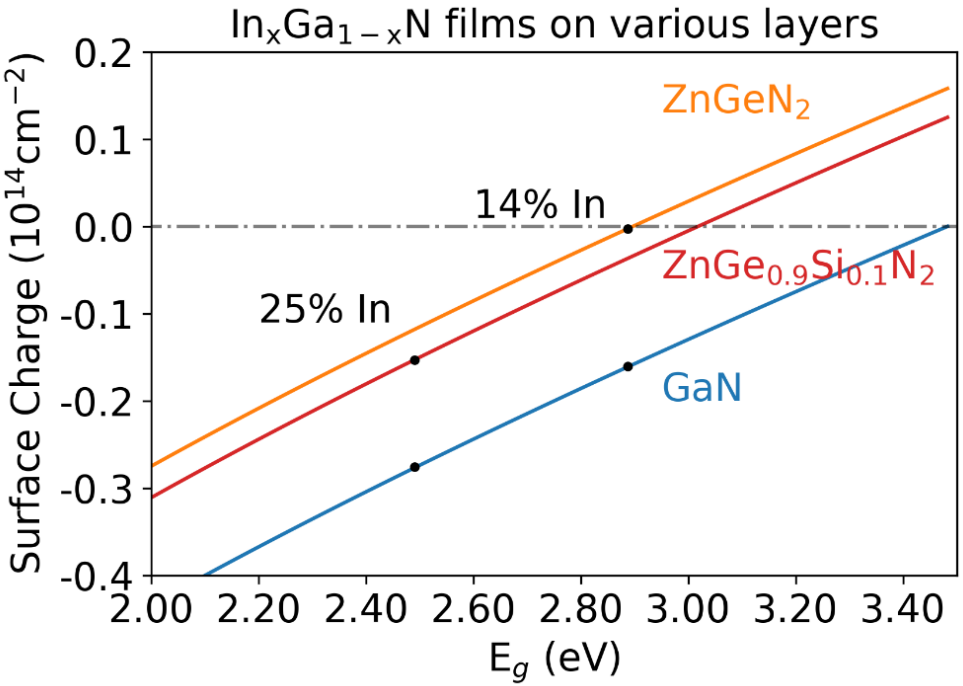


$In_xGa_{1-x}N$ / $ZnGeN_2$ polarization charge goes to zero near 14% In

- Issue: confinement

Bound charges at strained interfaces

$$\sigma_b = (P_{SP}^m - P_{SP}^n) - \epsilon_1 \left(e_{31}^n - e_{33} \frac{C_{13}^n}{C_{33}} \right) - \epsilon_2 \left(e_{32}^n - e_{33} \frac{C_{23}^n}{C_{33}} \right)$$



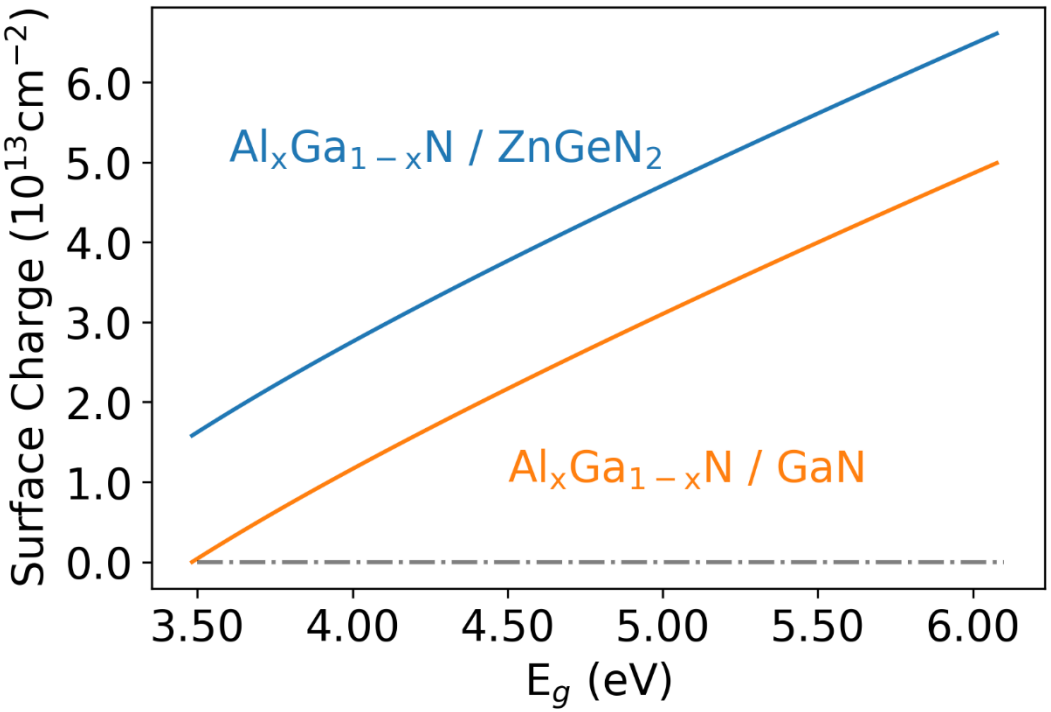
$In_xGa_{1-x}N$ / $ZnGeN_2$ polarization charge goes to zero near 14% In

- Issue: confinement
  - ➢ Use $ZnGe_{1-x}Si_xN_2$ alloys to increase CB offset

$In_{0.25}Ga_{0.75}N$ / $ZnGe_{0.9}Si_{0.1}N_2$ polarization charge 40% less than for InGaN/GaN interfaces

$AlGaN/ZnGeN_2$ interfaces

- $AlGaN/ZnGeN_2$ interfaces have increased polarization charge compared to AlGaN/GaN interfaces
- Type-II offset increases $\Delta CBM\ offsets by 0.5\ eV$



Conclusions

- II-IV-Nitrides can be integrated with III-Nitrides
- $ZnGeN_2$ can be dopable *n* or *p* type
- $ZnGeN_2$ has a type-II band offset with GaN
- Polarization engineering possible with heterostructures between III-Nitrides and II-IV-Nitrides