SAND2022-6755C

University Partnerships (UP) Supplemental Project 222547 Report – FY22 Q*x*

NMSU

Project Title: Defect Mediated and Diode Degradation in Wide Band-Gap AlGaN Electronics

University Partnerships
Sandia Academic Alliance, Campus Executive, START HBCU

Introduction and Motivation

Power Electronics:

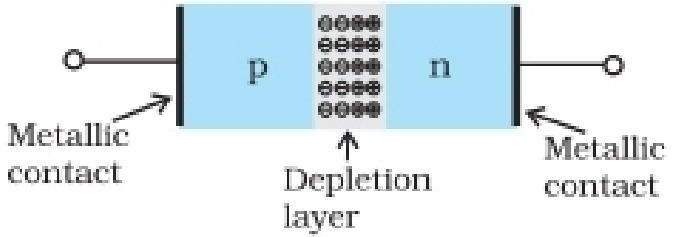
- Used to control and convert electric power, common in electronic consumer devices.
- Requires the use of high-efficiency, high-voltage transistors.
- AlGaN heterostructures have been used for PE designs for HEMT, RTDs, and more.
  - (Bayram et al., 2010)

Ultra-wide-bandgap ($E_{UV} \sim 3.1$ eV) **Uses of AlGaN:**

- Some aspects of diode performance can scale non-linear with increased band gap.
  - (Tsao et al., 2018)
- UV Light emitting diodes, photodetectors, ultra-fast "switch" for power electronics, high-temperature and high-power durability.
  - (Li et al., 2017; Lebedev, 1999; Hudgins et al., 2003; Chow, 1994)
- Amplifiers of high current electronic devices.

AlGaN Based Surfaces and Interfaces:

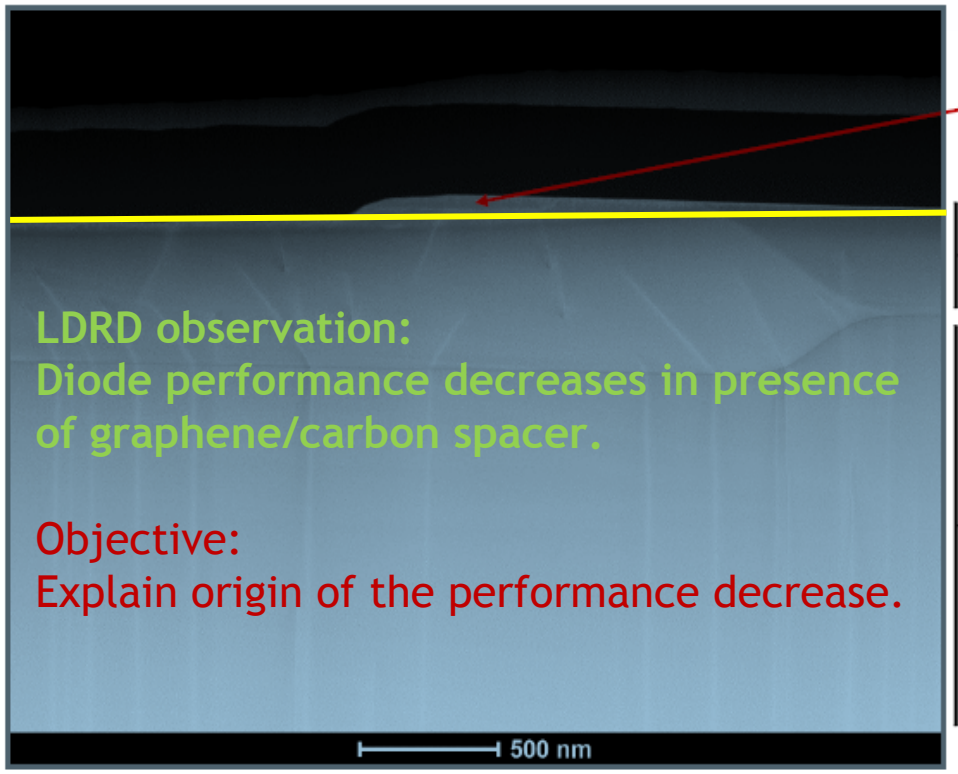
- p-n Interface preferability
- Surface Metallicity
- Carbon interface influence and amorphization



Semiconductor diode, (toppr.com)

Introduction and Motivation:

Experiment (LDRD) ➔ Theory



P-GaN

Regrown p-30% AlGaN

N- 31% AlGaN

Mg-GaN

graphene/carbon "spacer".
Mg-AlGaN.

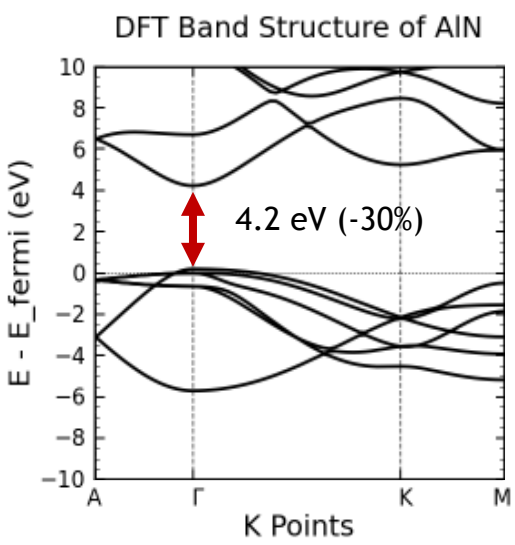
Si-AlGaN

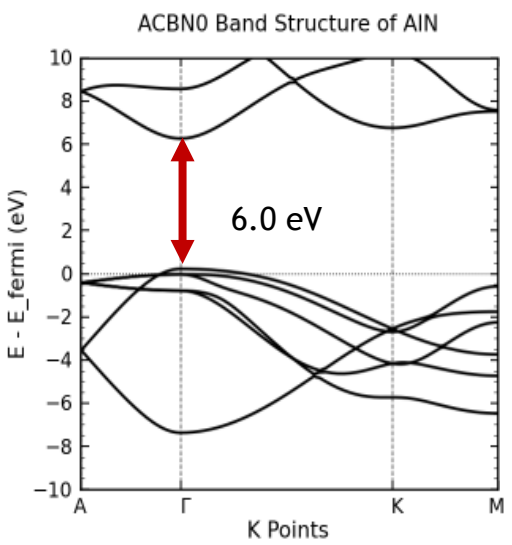
Diode Substrate

Computational Approach: All calculations were completed using Quantum Espresso Software Package (Giannozzi et al., 2017) .

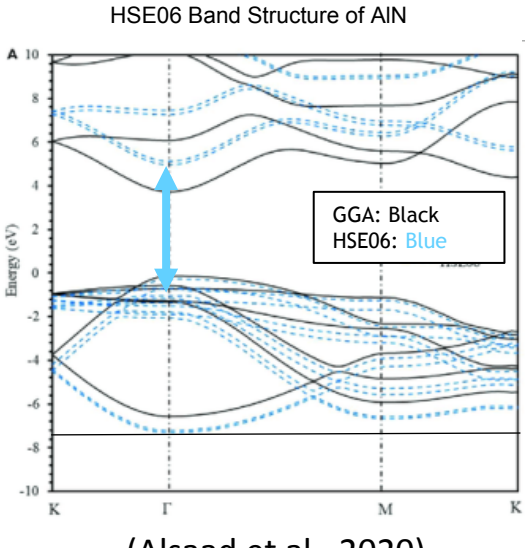
- Density Functional Theory (DFT).
- Generalized gradient approximation.
  - (Perdew et al., 1996)
- DFT-like ACBN0 approach increases DFT band gaps.
  - (Agapito et al., 2015)
- Computations are largely optimized for an energy cutoff of 75 Ry, and K-point sampling of 6x6x4 for a bulk, 4-atom unit cell.
- E_g converged to 0.02 eV

This work





Exp.: 6.026 eV (Guo and Yoshida, 1994)



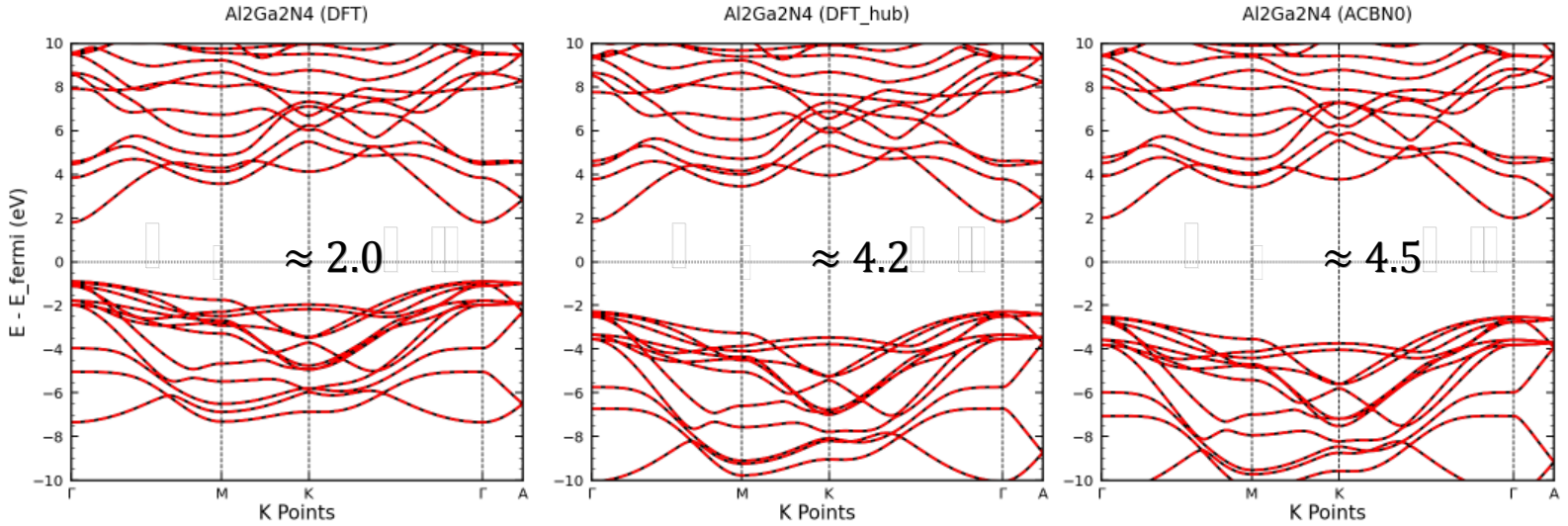
(Alsaad et al., 2020)

Results:

- ACBN0 increases DFT bandgap as expected.
- Comparable to experiment and resource demanding HSE06 computations.

Improving Reliability of ACBN0 Computations

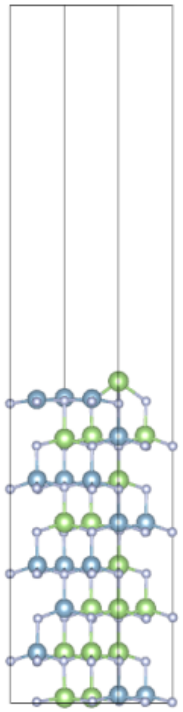
	DFT_hub	Experiment
AlN	5.74 eV	6.2 eV (Yim et al., 1973)
GaN	3.19 eV	3.39 eV (Maruska, 1969)
AlGaN	4.18 eV	4.5 eV (Sang et al., 2013)



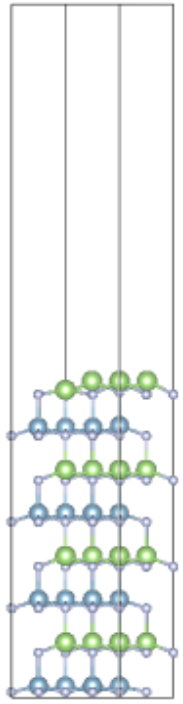
Thermochemistry	DFT	DFT	ACBN0
Electronic Structure	DFT	ACBN0	ACBN0

- New Process: DFT vc-relax → Add H-U Parameters → Band Structures **(without re-relaxing)**
- The new process relaxed structure sees a -1.4% deviation in the lattice parameters from true ACBN0.
- New process produces a similar band gap and does not require the unknown Hubbard-U parameters of required atomic species.

Technical Accomplishments and Updates: Ordered vs Disordered

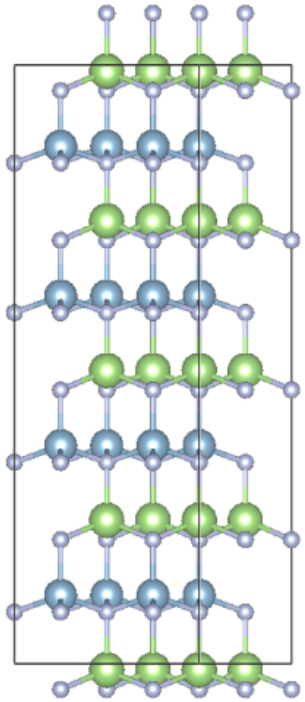


Disordered:
ΔE = +7.29 meV/atom

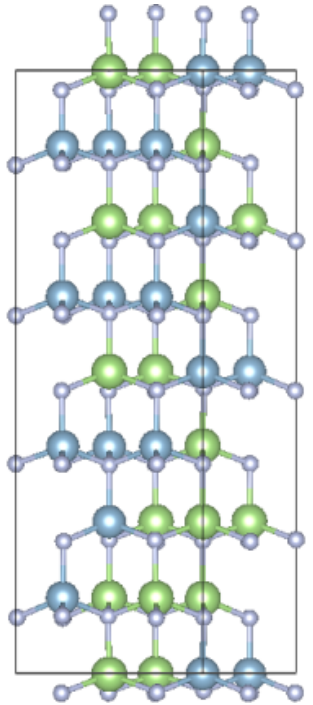


Ordered:
ΔE = 0 eV/atom

Same composition



Ordered:
ΔE = +3.4 meV/atom



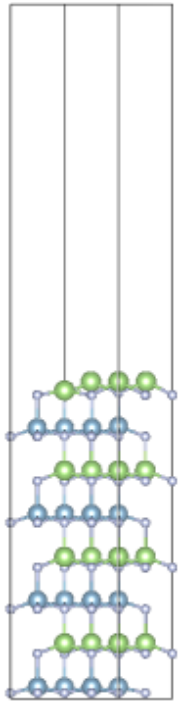
Disordered:
ΔE = 0 eV/atom

Same composition

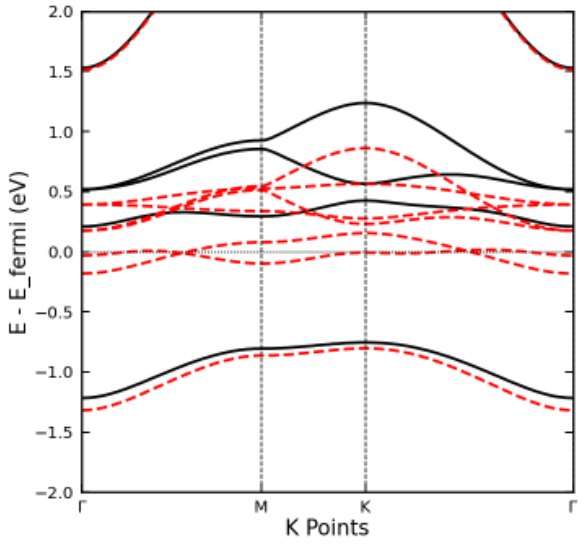
- Ga truncation is more energetically favorable than the Al truncations for surface calculations.
- Disordered AlGaN may perform better in strain-based scenarios due to the uniform strain distribution (Cheng et al., 2019) .

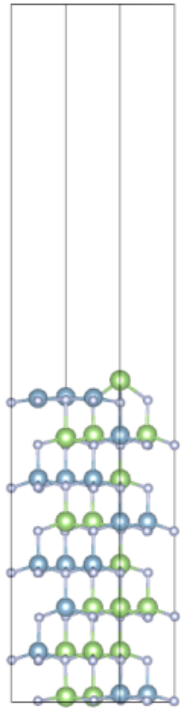
- **Bulk and Disordered structures are energetically near generate, $\Delta E < 25 \frac{meV}{atom}$.**

Technical Accomplishments and Updates: Metallic surfaces

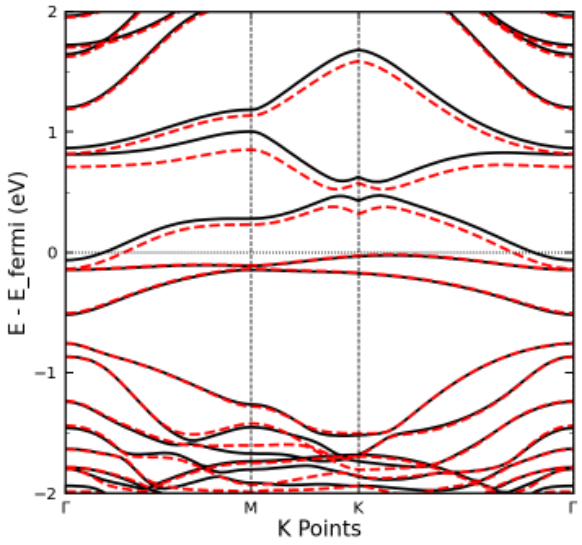


8-layer, 64-atom





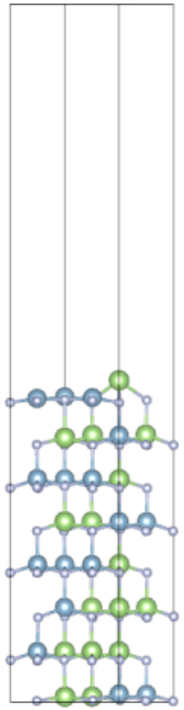
8-layer, 64-atom



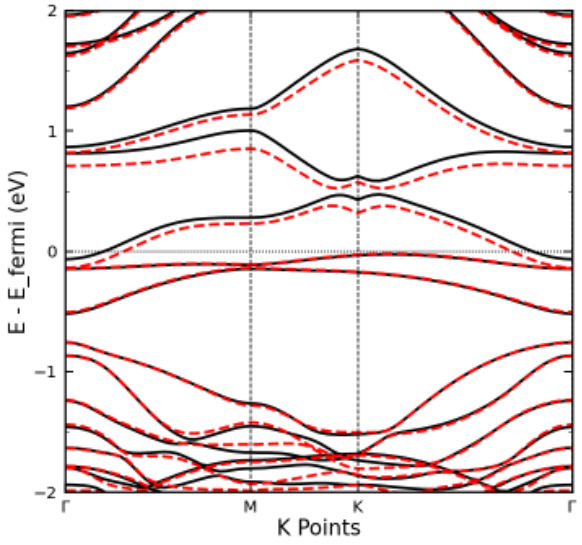
- Bulk AlGaN is a widegap material, $E_g = 4.5\ eV$.
- Many-layered AlGaN slabs are metallic, implying that creating interfaces would reduce diode performance.

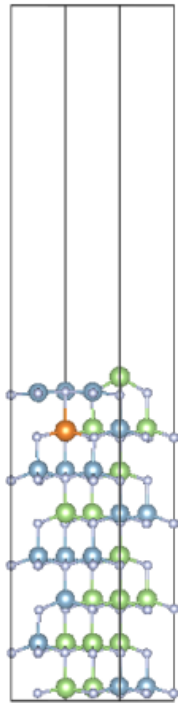
- **Unbound electrons at surface are delocalized and conducting → Forming surfaces closes the bandgap.**
- **Forming an interface and filling the vacuum will create new bonds, reopening the bandgap.**

Technical Accomplishments and Updates: Metallic surfaces

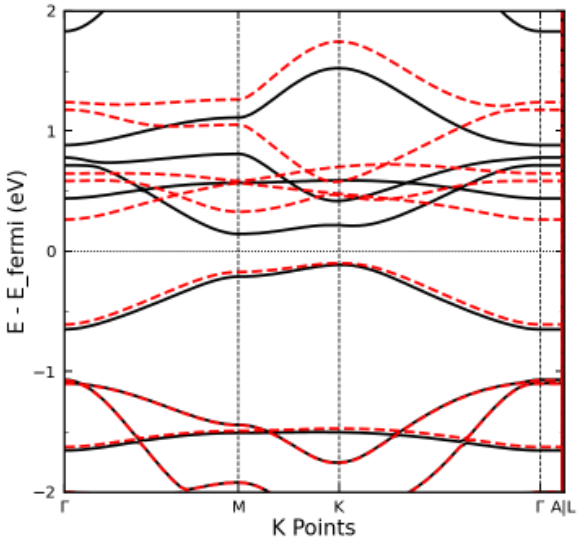


8-layer, 64-atom





8-layer, 64-atom, Ga ➔ Mg

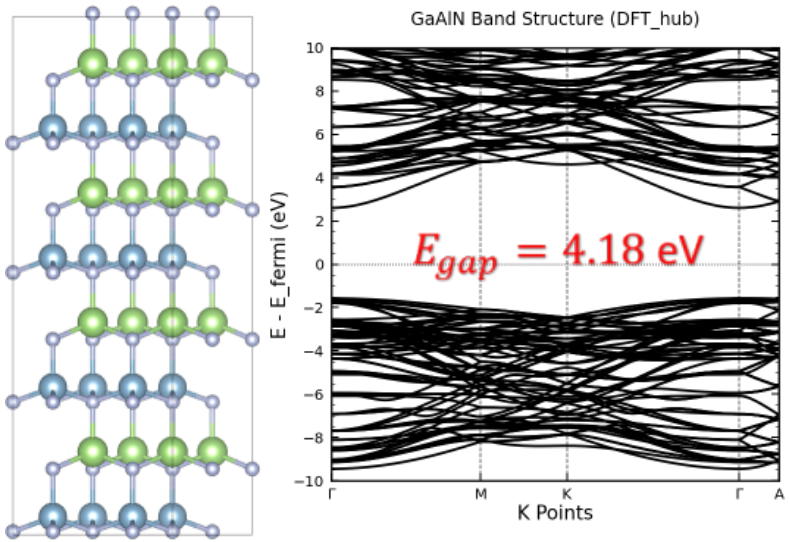


- Subsurface doping shows an opening of the band gap ➔ $E_g = 0.24$ eV.
- Unbound orbitals along the surface may partially fill p-type electron hole.
- ΔE_{form}= −86 meV from next most favorable dopant location.

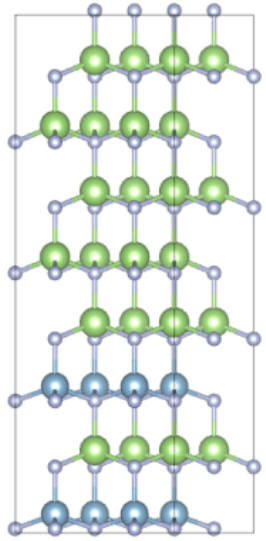
- **Electron conducting diodes may see increased performance by countering with electron holes.**
- **Hole + electron ➔ p-n heterojunctions are predicted to perform well.**

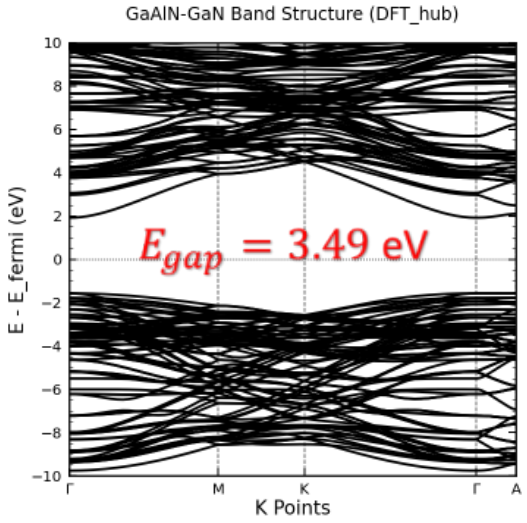
Technical Accomplishments and Updates: Insulating Interfaces

- At this point that we shifted our attention to the experimental interfaces developed by the LDRD team.
- Computational methods resolve average CBM for AlGaN, GaN, and AlGaN/GaN ~2.0 eV, agreeing with experiment (Kim et al., 2019)
.

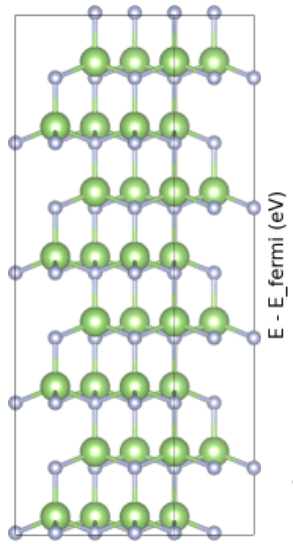


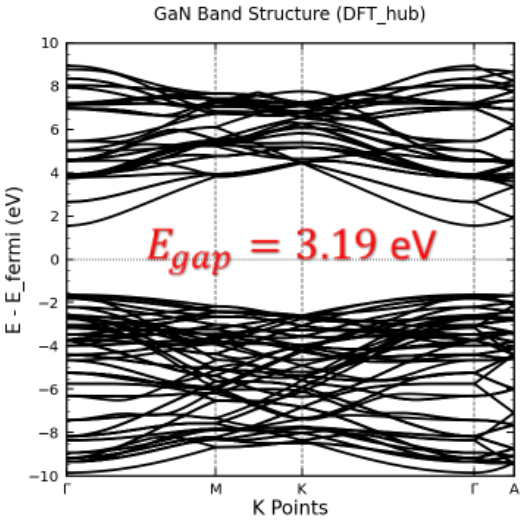
Strain: +0.73%





Strain: +1.46%





Exp: 4.5 eV (Sang et al., 2013)

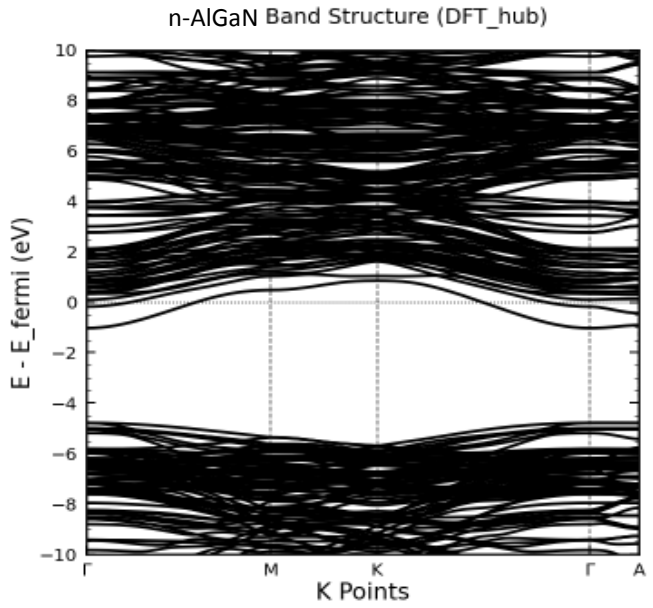
Within accepted parameters (Ekpunobi, 2002).

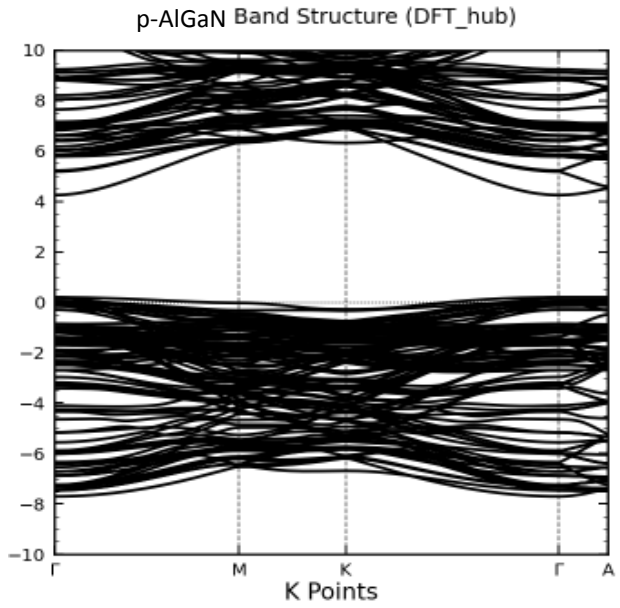
Exp: 3.39 eV (Maruska and Tietjen, 1969)

- **Results: Closing the gap above a surface will fill the open orbitals, recreating an insulating material.**
- **The heterostructure gap is noticeably near the average of the two separate bulk structures.**

Technical Accomplishments and Updates: n-AlGaN/p-AlGaN Interface Favorability

- The focus was on three diode compositions: p-AlGaN/p-GaN, AlGaN/p-GaN, and p-AlGaN/n-AlGaN (Carbon omitted for computation).
- Due to the extra electrons in p-type heterojunctions, p-AlGaN/p-GaN and AlGaN/p-GaN interfaces are localized hole conductors, leading to endothermic alloying energies and a metallic band gap.
- n-AlGaN/p-AlGaN heterostructures are computed as widegap insulators, suitable for diode production.

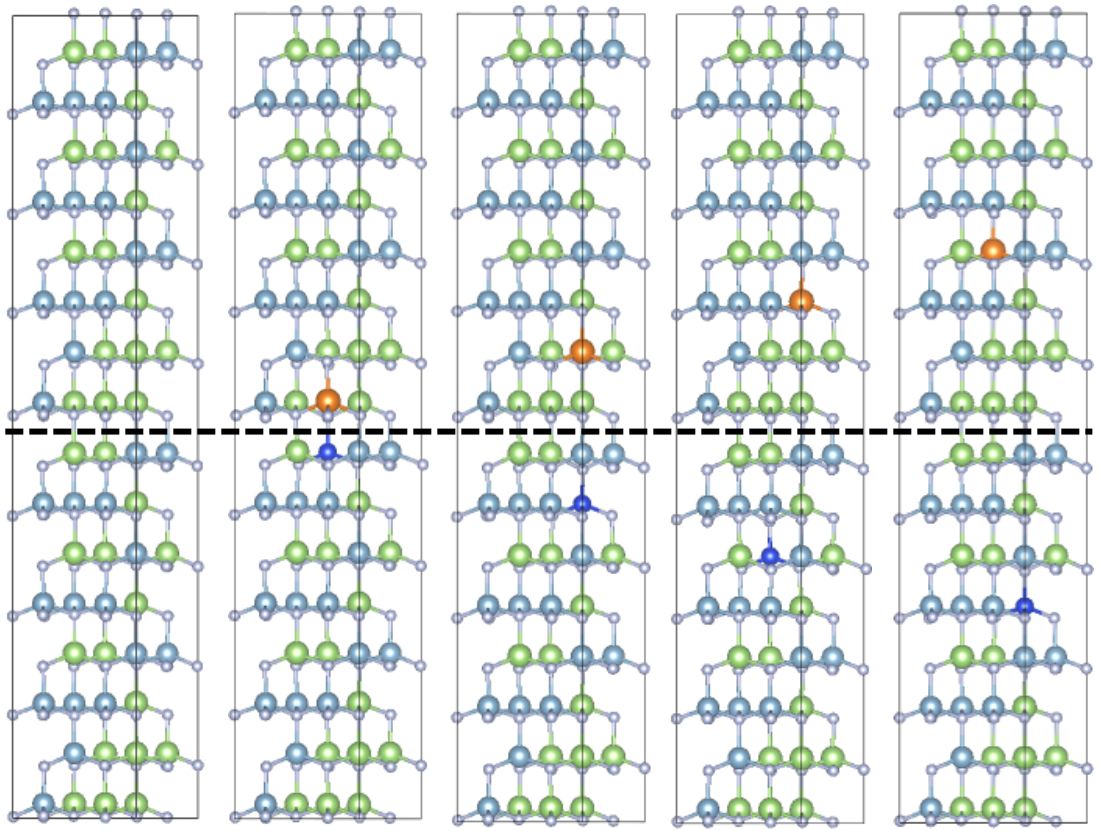




- n-AlGaN: Conduction band metallic, $E_{gap} = N/A$.
- p-AlGaN: Valence band metallic, $E_{gap} = 4.06\ eV$.
- Mg-doping shifts VBM upwards as expected.
  - (Li and Kang, 2007)

Expectation:
n-type electron donor + p-type electron hole
➔ Insulating heterostructure

Technical Accomplishments and Updates: n-AlGaN/p-AlGaN Interfaces

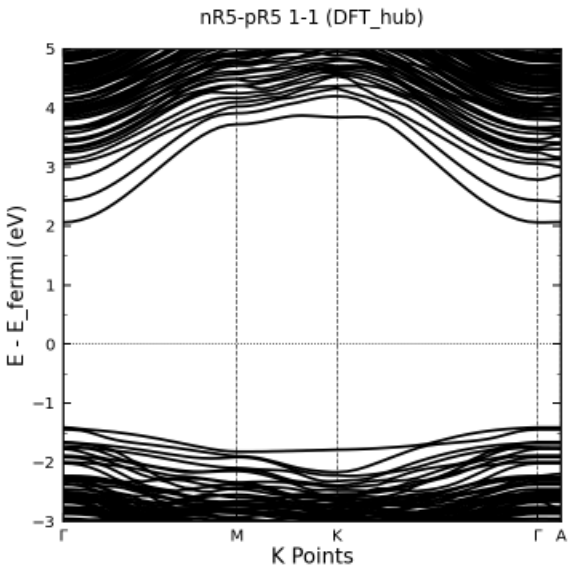


Distance Dependence

Distance From Interface	Alloying Energy	Fundamental Gap
$\Delta z_{Average}$ = 0.13 nm	-1.059 eV	3.472 eV
$\Delta z_{Average}$ = 0.39 nm	-0.036 eV	1.556 eV
$\Delta z_{Average}$ = 0.65 nm	0.302 eV	Metallic
$\Delta z_{Average}$ = 0.90 nm	0.788 eV	Metallic
AlGaN (Undoped)	E_g = 4.242 eV	

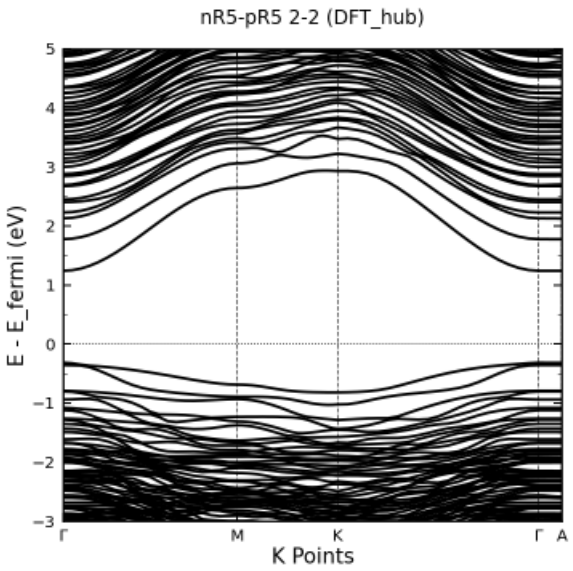
- Hole + electron creates insulating material in agreement with similar p-n band offsets.
  - (Lang et al., 1987)
- Coulomb interactions and strain overlap may increase band gaps and decrease alloying energies.
- **Dopants accumulate near the interfaces; near interface doping may increase diode performance.**

Technical Accomplishments and Updates: n-AlGaN/p-AlGaN Interfaces



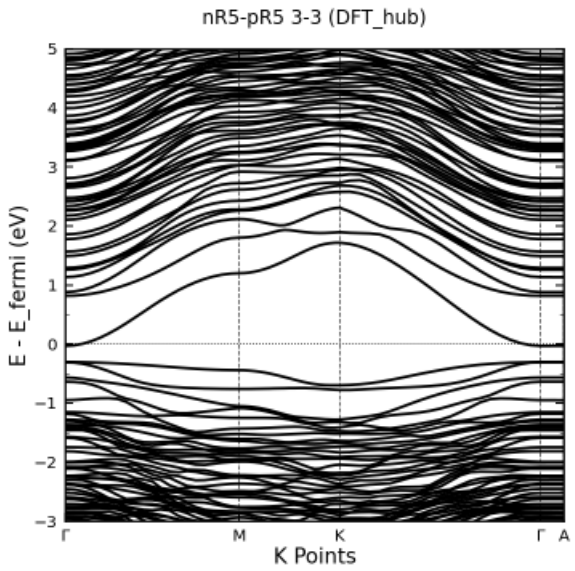
$\Delta z_{avg} = 0.13$ nm

$\Delta E_{form} = -1.06$ eV



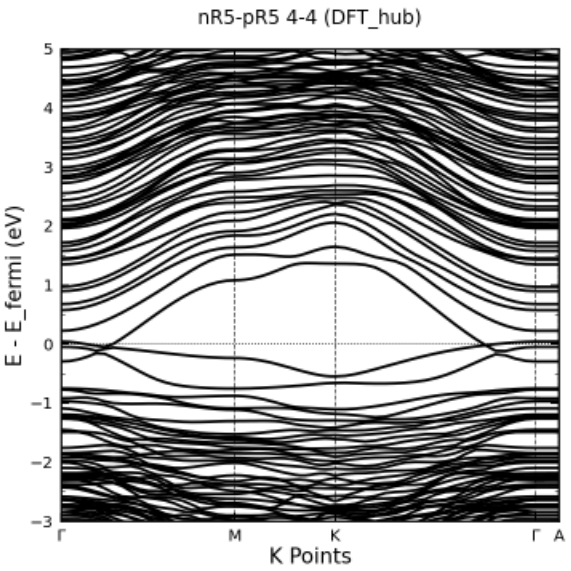
$\Delta z_{avg} = 0.39$ nm

$\Delta E_{form} = -0.04$ eV



$\Delta z_{avg} = 0.65$ nm

$\Delta E_{form} = 0.30$ eV



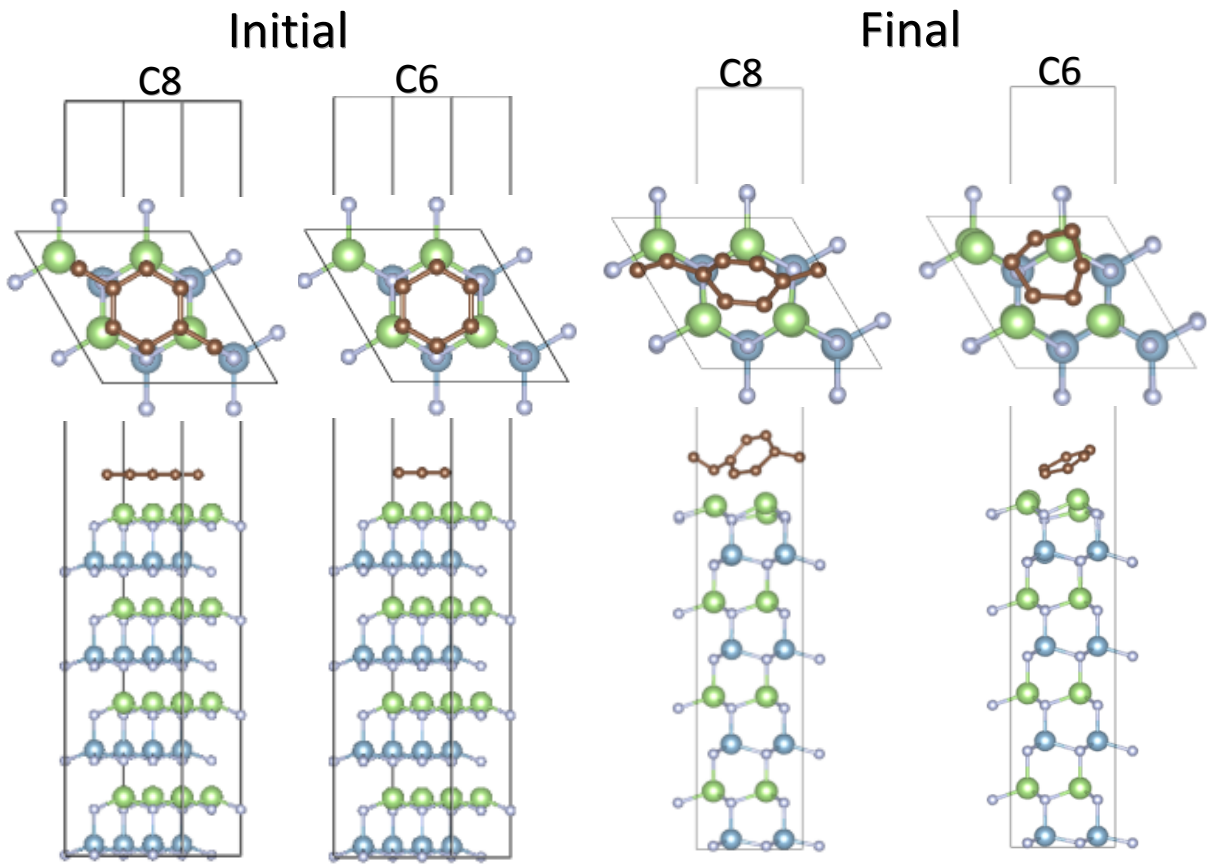
$\Delta z_{avg} = 0.90$ nm

$\Delta E_{form} = 0.79$ eV

Lower — Distance From Interface, Alloying Energy, Metallicity — Higher

Technical Accomplishments and Updates: Metallic Surfaces with Carbon, Carbon Amorphization

- **First attempts at introducing carbon to an Ordered AlGaN interface:**



Std Dev. Initial C-C Graphene bonds: 0.001 (Å)

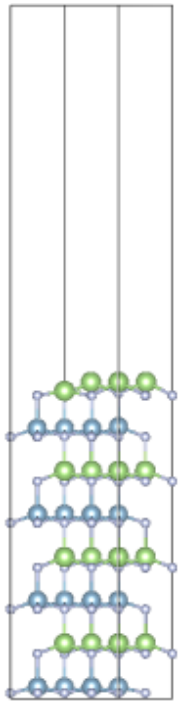
	C8: Std Dev.	C6: Std Dev
Undoped	0.078 (Å)	0.050 (Å)
Doped	0.076 (Å)	0.069 (Å)

Insights:

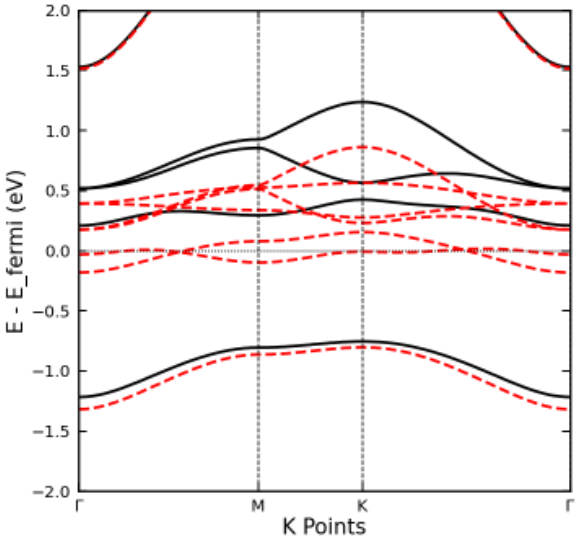
- 8-atom and 6-atom carbon molecules both appear to be amorphous.
- Carbon molecules experience torque.
- Testing included p-doped surfaces.

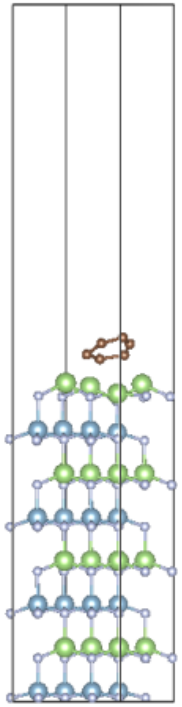
Conclusion:
C-C edges may cause amorphization at ordered AlGaN surfaces/interfaces, independent of doping.

Technical Accomplishments and Updates: Effect of C6 ring of Ordered AlGaN

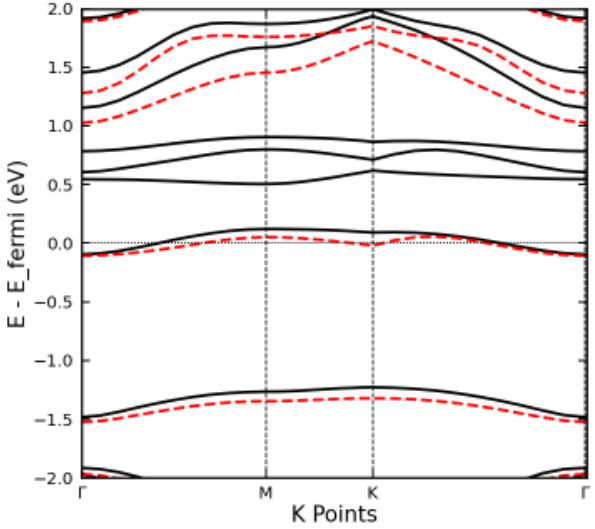


8-layer, 64-atom AlGaN





AlGaN/C6 Surface

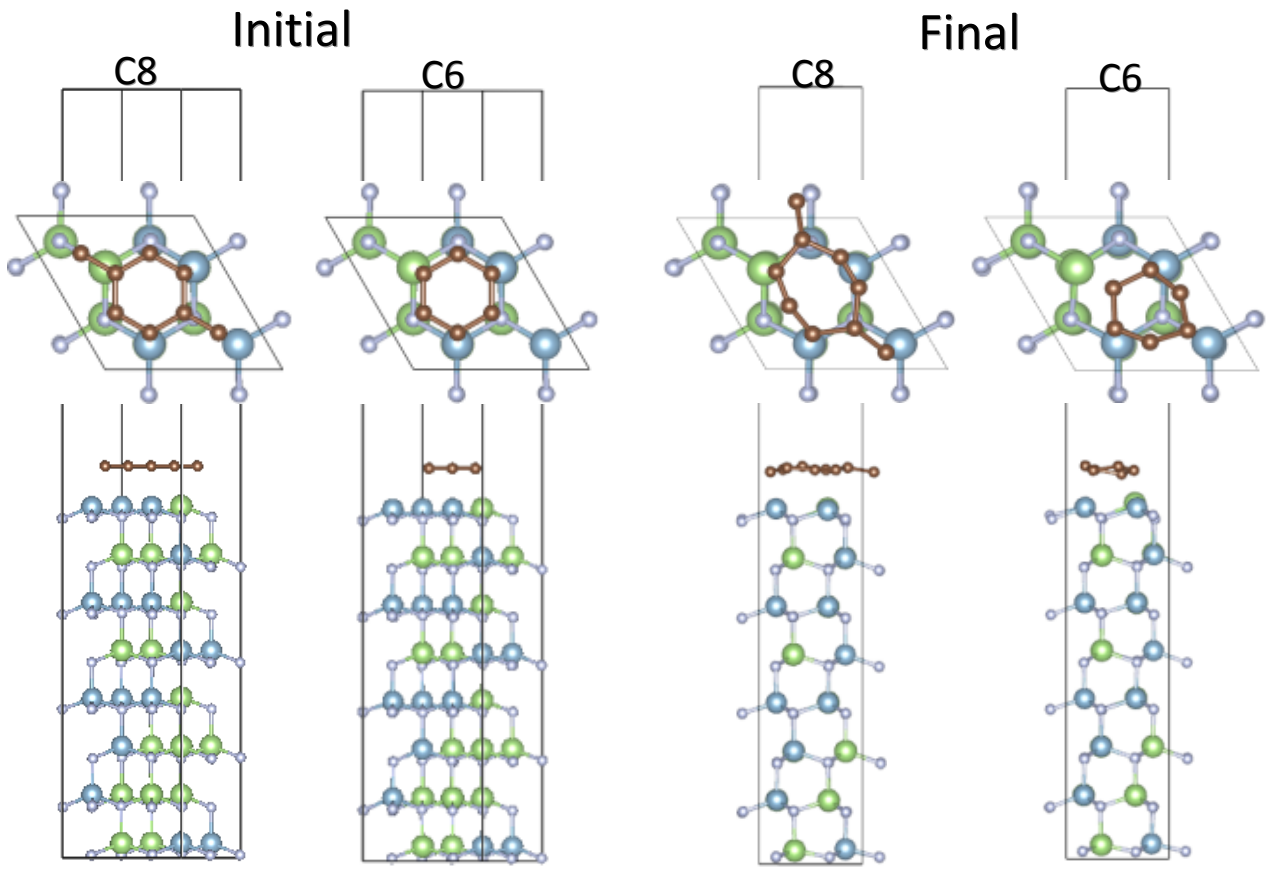


- The carbon spacer does little to mediate the metallicity of the surfaces.
- Carbon induces slight amorphization in AlGaN substrate, likely due to sp2 carbon orbitals.

- **Carbon molecules interact with the substrate, changing the density of near-fermi level bands**
- **Carbon does not affect metallicity or increase diode performance.**

Technical Accomplishments and Updates: Metallic Surfaces with Carbon, Carbon Amorphization

- **First attempts at introducing carbon to a Disordered AlGaN interface:**



Std Dev. Initial C-C Graphene bonds: 0.001 (Å)

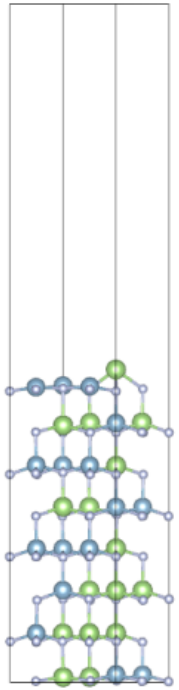
	C8: Std Dev.	C6: Std Dev
Undoped	0.096 (Å)	0.051 (Å)
Doped	0.074 (Å)	0.065 (Å)

Insights:

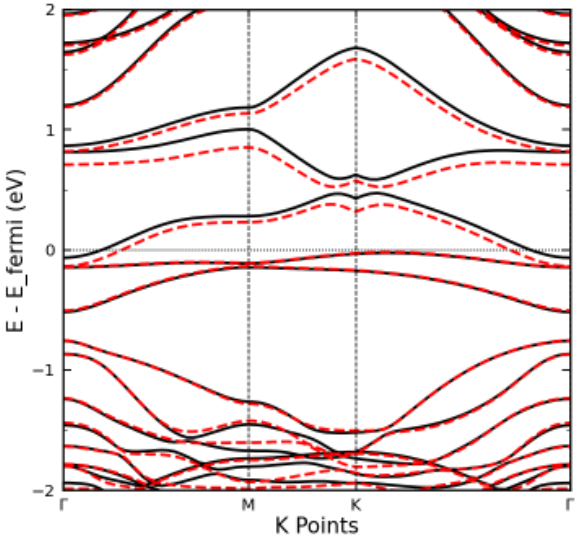
- 8-atom and 6-atom carbon molecules appear to be amorphous and experience a torque.
- Disordered distributions see reduced z-axis buckling.

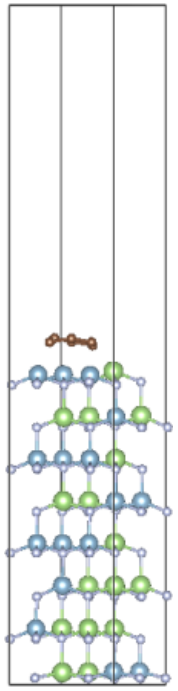
Conclusion:
C-C edges may induce amorphization, amorphization is relatively consistent between ordered and disordered AlGaN.

Technical Accomplishments and Updates: Effect of C6 ring of Disordered AlGaN

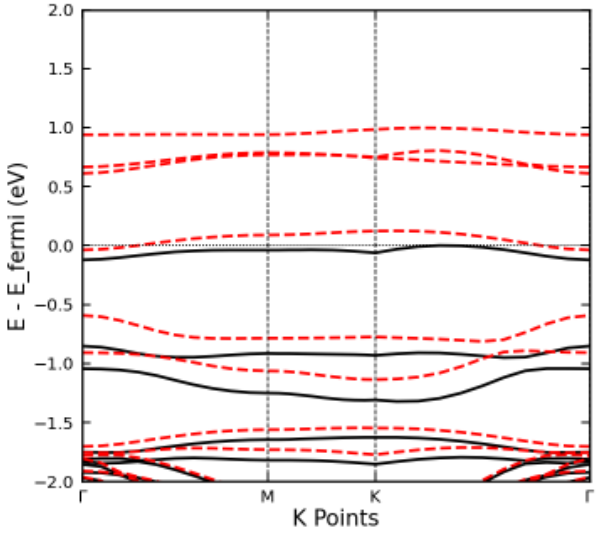


8-layer, 64-atom





AlGaN/C6 Surface



- The carbon spacer does little to mediate the metallicity of the surfaces.
- Disordered substrate is more uniform than ordered substrate, likely due to uniform strain distribution.

- **Carbon molecules interact with the substrate, changing the density of near-fermi level bands**
- **Carbon does not affect metallicity or increase diode performance.**

Conclusions:

- Devices based on AlGaN, GaN or their interfaces show great potential for high-power, high-temperature, and high-frequency power electronics due to the nature of wide-band gap semiconductors.
- Enhanced the widely used Density Functional Theory computational method using ACBN0 to increase the accuracy of our calculated electronic properties of wide gap semiconductors.
- Our results show bulk AlGaN is a good insulator, AlGaN surfaces destroy diode insulation.
- Non-metallic p-AlGaN (disordered) surface suggest localized hole-conductors, and uniform strain distribution reopening the band-gap.
- p-n AlGaN diodes are promising → hole + electron conduction open band gap, dopants accumulate near interface.
- Localized carbon molecules have a benign effect on the electronic properties of AlGaN substrates.
- Carbon becomes amorphous, roughly 50x that of unperturbed graphene, strongly suggesting that C-C edges induce amorphization.