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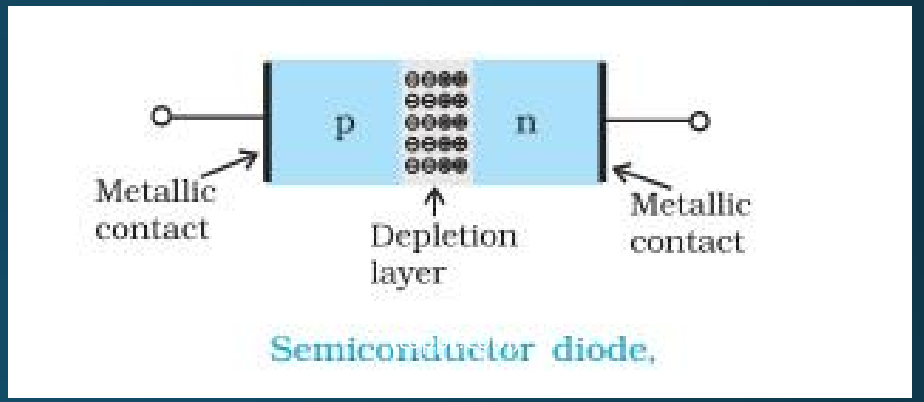
Material Properties of Widegap AlGaN for use in Power Electronics

Authors: Nicholas Baldonado (PhD Student), Dr. Boris Kiefer (New Mexico State University), Dept. of Physics, Dr. Julia Deitz (SNL)

Introduction and Motivation

Power Electronics

- Used to control and convert electric power, common in electronic consumer devices.
  - Can convert currents between AC/DC.
  - Used in household electronics, chargers, batteries, etc.
- Requires the use of high-efficiency, high-voltage transistors.
- AlGaN material may be optimal for creating transistors and diodes.
  - p-n junctions (diodes) require finite band gap.
  - Mg dopant: electron acceptor (p-type).
  - Si dopant: electron donor (n-type).



Properties and Applications of AlGaN:
Undoped and doped:

- Wide band gap: UV Light emitting diodes, photodetectors.
- Wide band gap: ultra-fast “switch” for power electronics.
- Amplifiers of high current electronic devices.

Doped AlGaN:

- High electron mobility transistor through modulation-doped heterojunction.
  Separation of dopant layer and mobility layer.
  ➔ reduced impurity scattering.
  ➔ increased energy/power efficiency.

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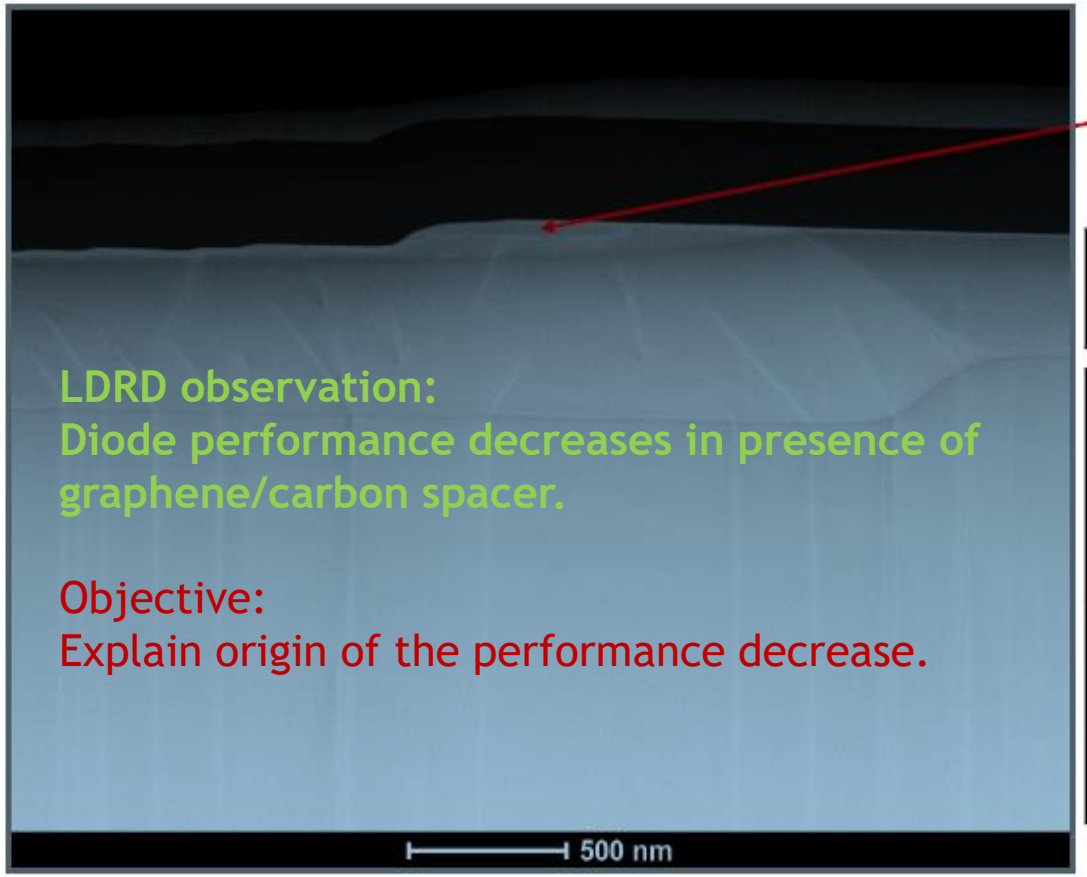
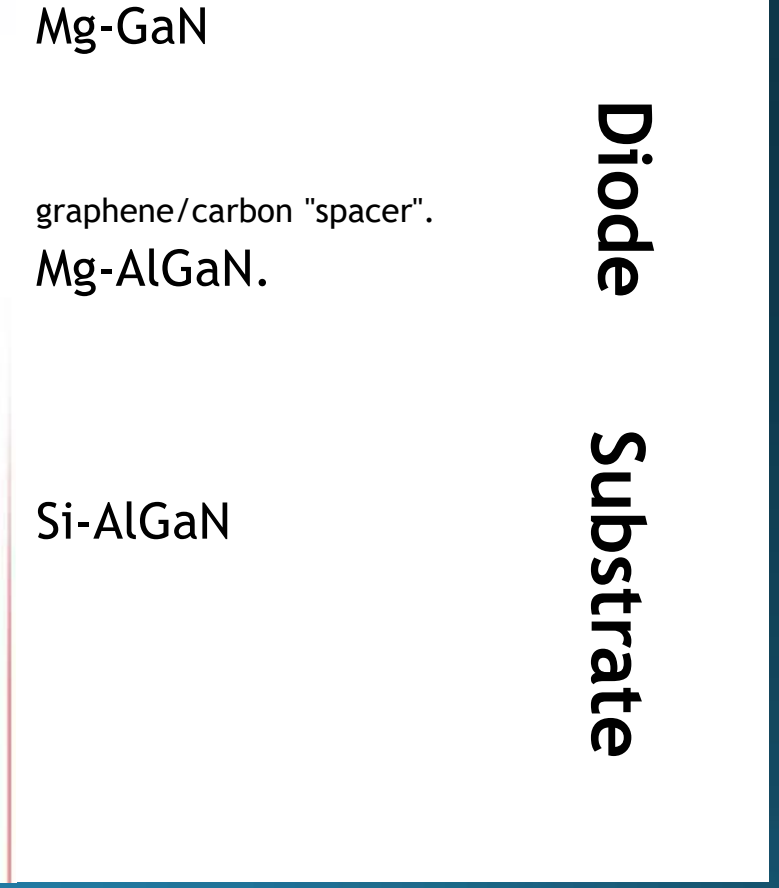
Introduction and Motivation

Experiment (LDRD) ➔ **Theory**



LDRD observation:
Diode performance decreases in presence of graphene/carbon spacer.

Objective:
Explain origin of the performance decrease.



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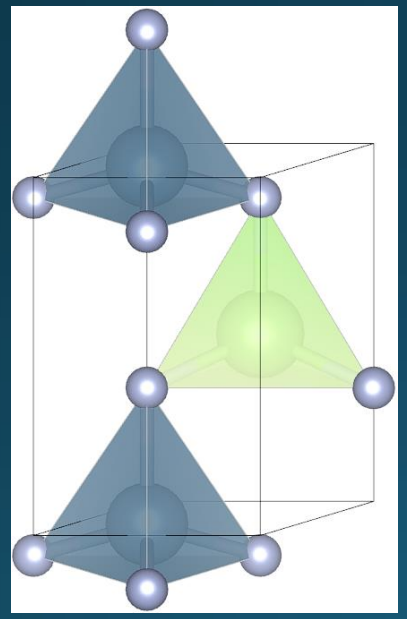
Computational Approach

Known Crystal Structure:

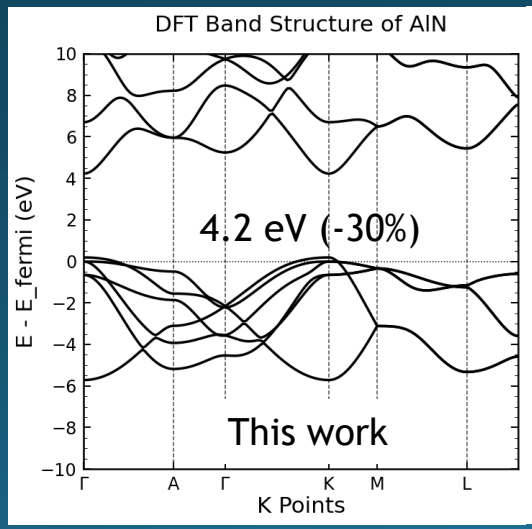
- Hexagonal (equilibrium phase).
- Ferroelectric.
- Corner sharing tetrahedral network.



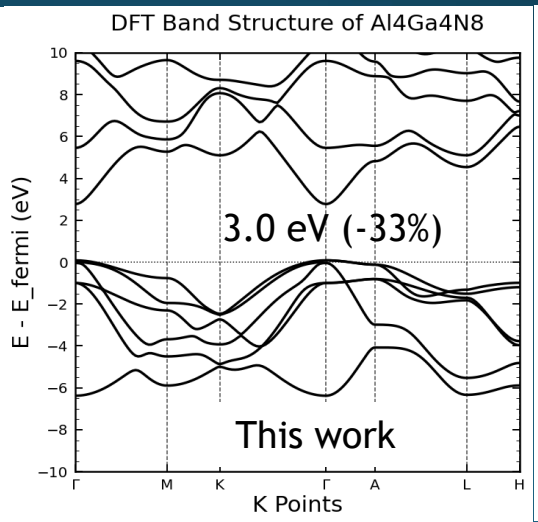
Quantum Espresso Software Package (Giannozzi et al., 2017)

- Density Functional Theory (DFT).
- Planewaves: Ecut = 70 Ry.
- K-points: 6 x 6 x 4.
- Generalized gradient approximation (PBE, Perdew et al., 1996).

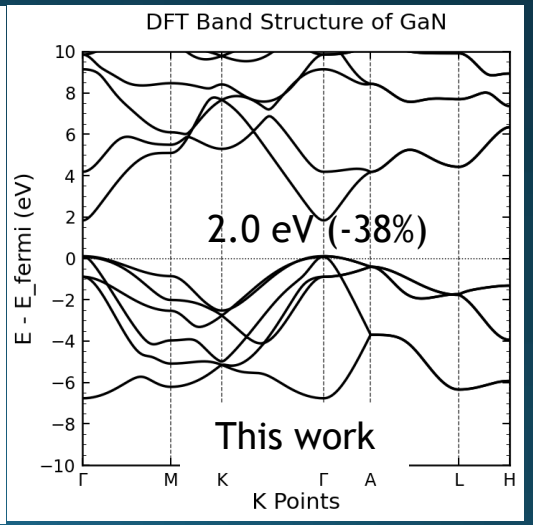
Exp.: 6.026 eV
(Guo and Yoshida, 1994)



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



Exp.: 3.2 eV
(Bougrov et al., 2001)



Insights: DFT systematically underestimates band gaps in materials.

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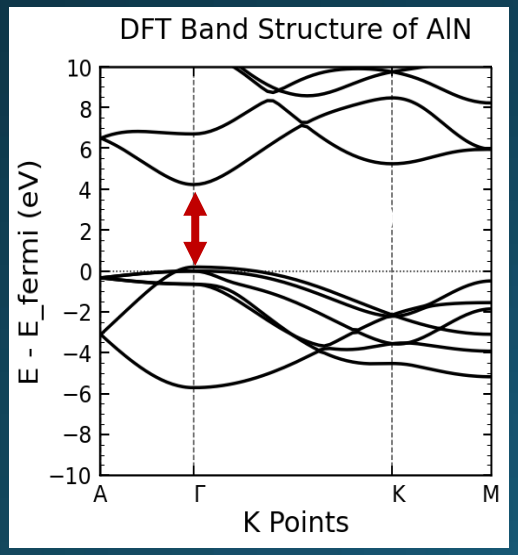
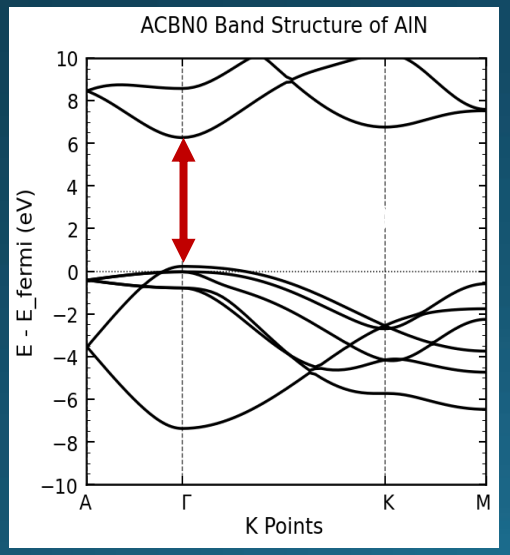
Computational Approach

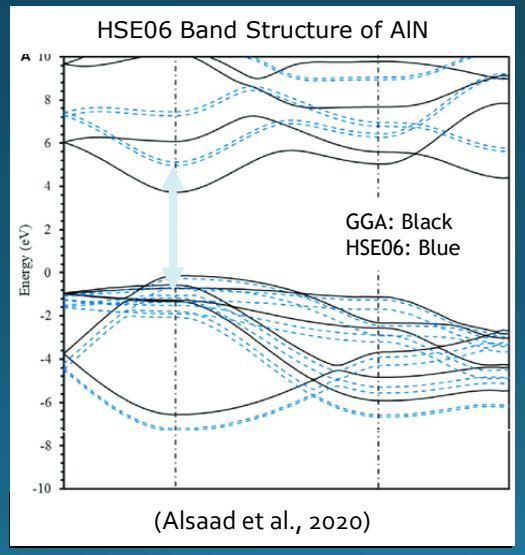
- DFT-like ACBN0 approach (Agapito et al., 2015) increases DFT band gaps.

	4-atom $AlGaN_2$	8-atom $AlGa_2N_4Mg$	16-atom $Al_3Ga_4N_8Mg$	8-atom Al_2GaN_4Mg	16-atom $Al_4Ga_3N_8Mg$	8-atom $AlGa_2N_4Si$	16-atom $Al_3Ga_4N_8Si$	8-atom Al_2GaN_4Si	16-atom $Al_4Ga_3N_8Si$
Al	0.0156	0.0079	0.0105	0.0171	0.0161	0.007	0.0197	0.0128	0.0159
Ga	18.121	18.088	17.587	17.95	17.992	17.978	18.051	18.01	18.429
N	4.973	5.049	5.037	6.917	5.255	4.537	4.664	5.077	4.733

This work







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

Results:

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

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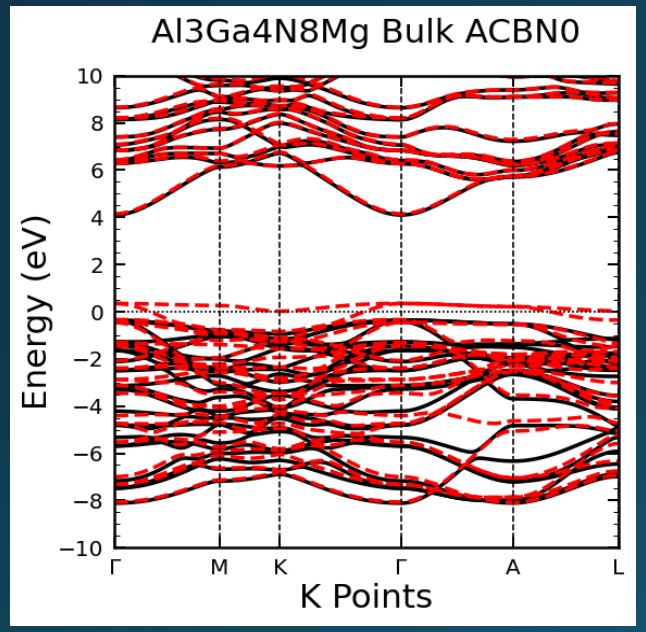
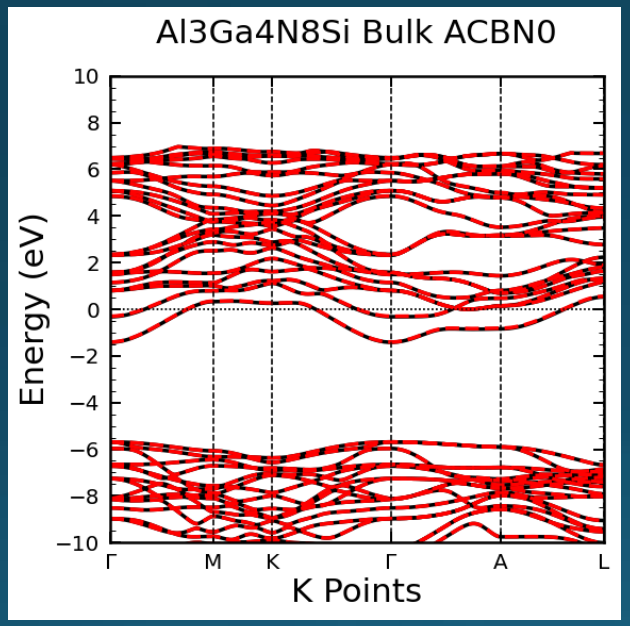
Doping Mg and Si in bulk AlGaN

p-type (Mg) doping

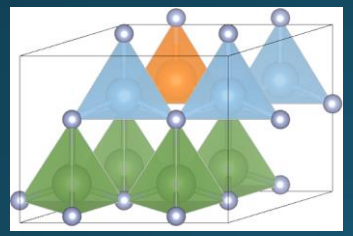


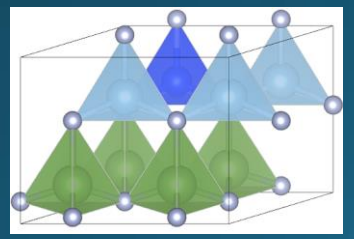
n-type (Si) doping

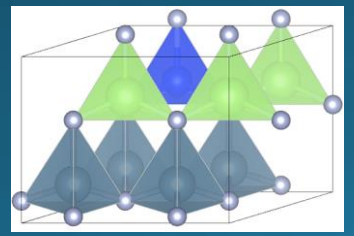


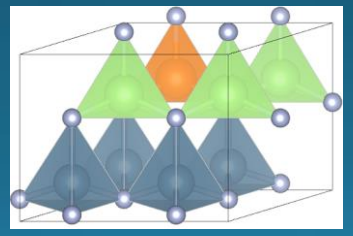
Results:

- Doped structures are metallic.
- Neither p-type nor n-type doping is thermodynamically favorable: $E_{Formation}$ > +0.5 eV.









➔ Mg and Si dopants accumulate on or near surfaces and interfaces.

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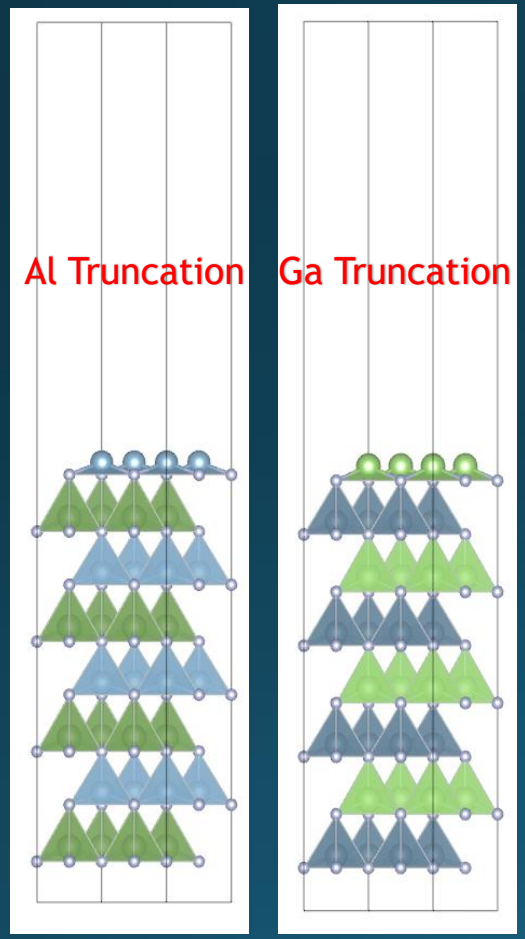
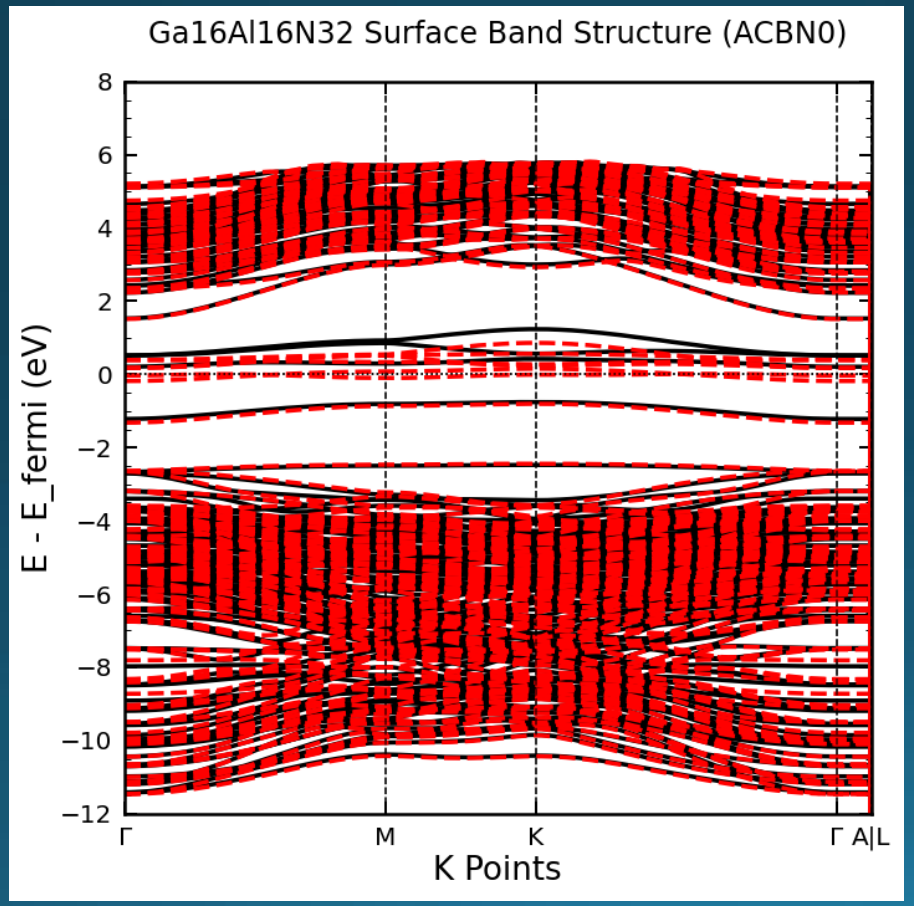
Surface Structure





Results:

- Surfaces structures are metallic.
- Metals ions remain non-magnetic.
- Nitrogen at bottom are magnetic (spin-polarized).

➔ **Possible explanation for LDRD observation.**

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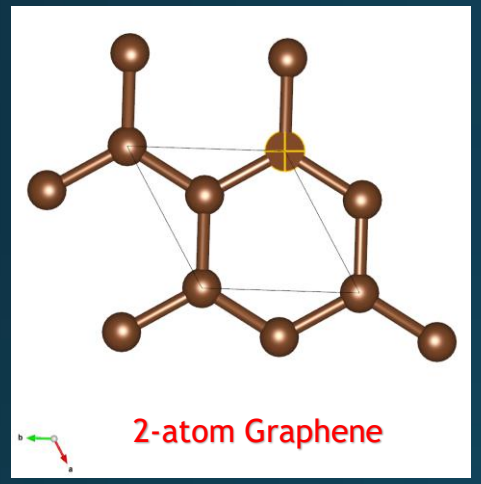
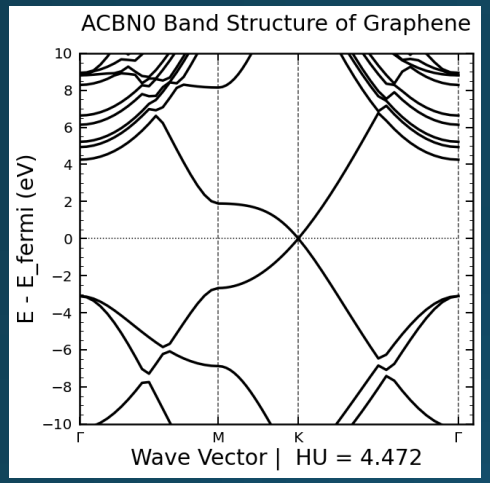
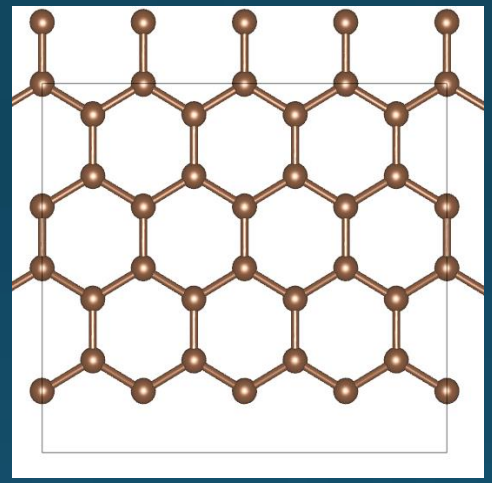
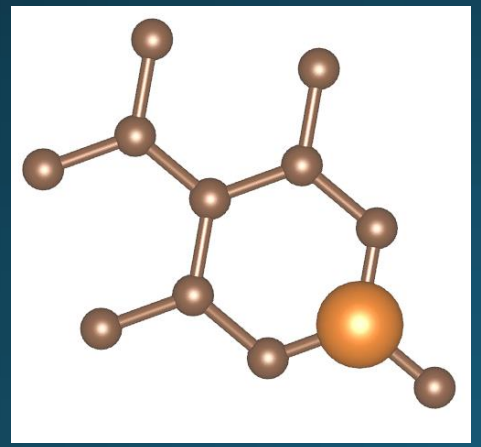
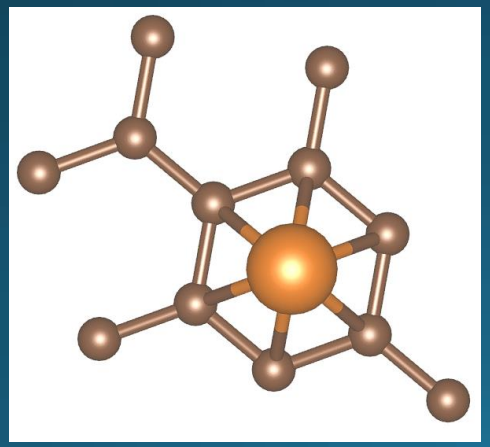
Graphene

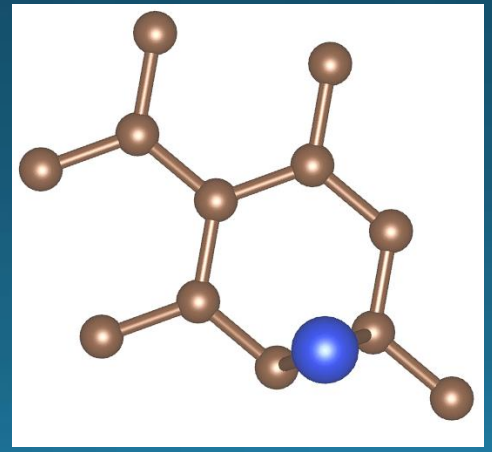












Results:

- Recovered well-known Dirac point in graphene.
- Mg distance > 3.5 A
  ➔ no bonding.
- Si distances < 2.5 A
  ➔ bonding.

Chemistry specific dopant graphene interactions.

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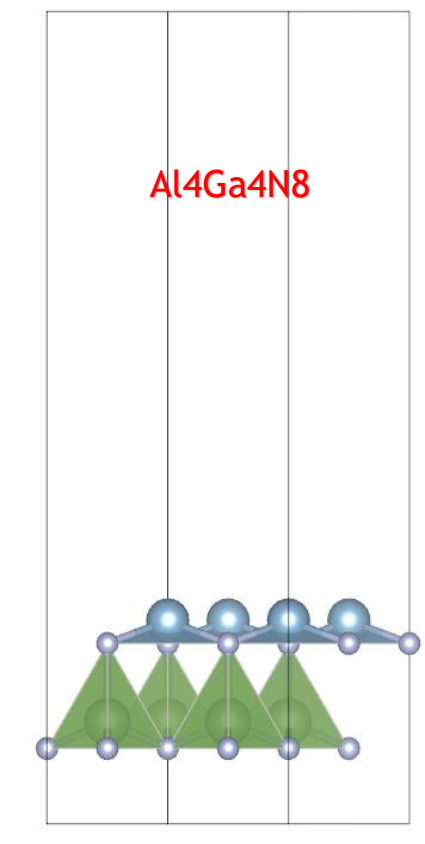
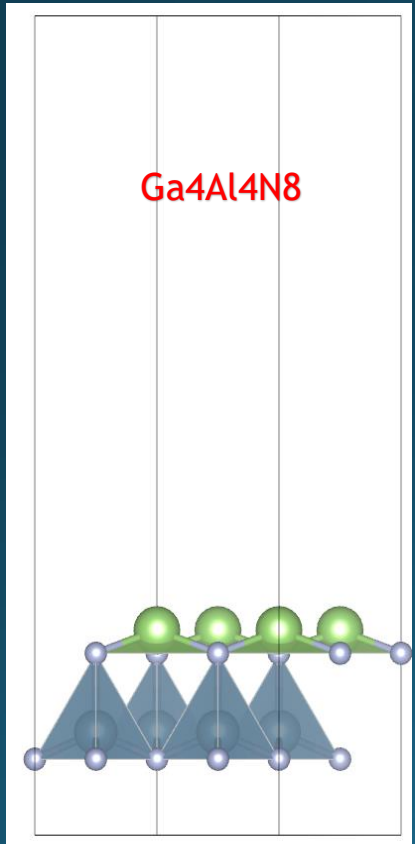
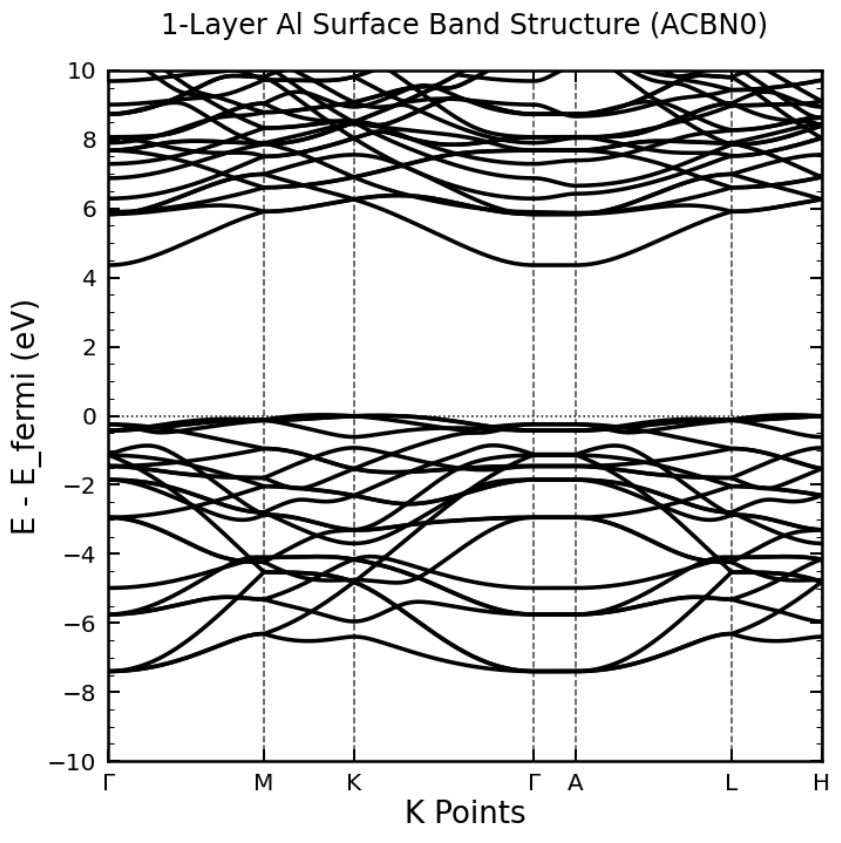
Monolayer AlGaN







Results:

- Stoichiometric monolayer remains insulating.
- Band gap comparable to bulk AlGaN.

➔ Surface available for dopants.

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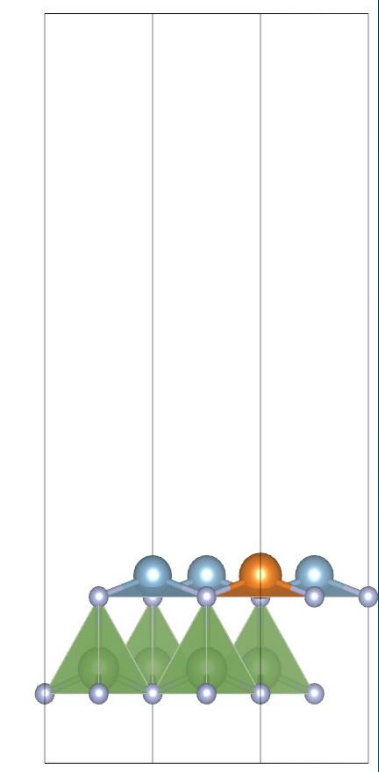
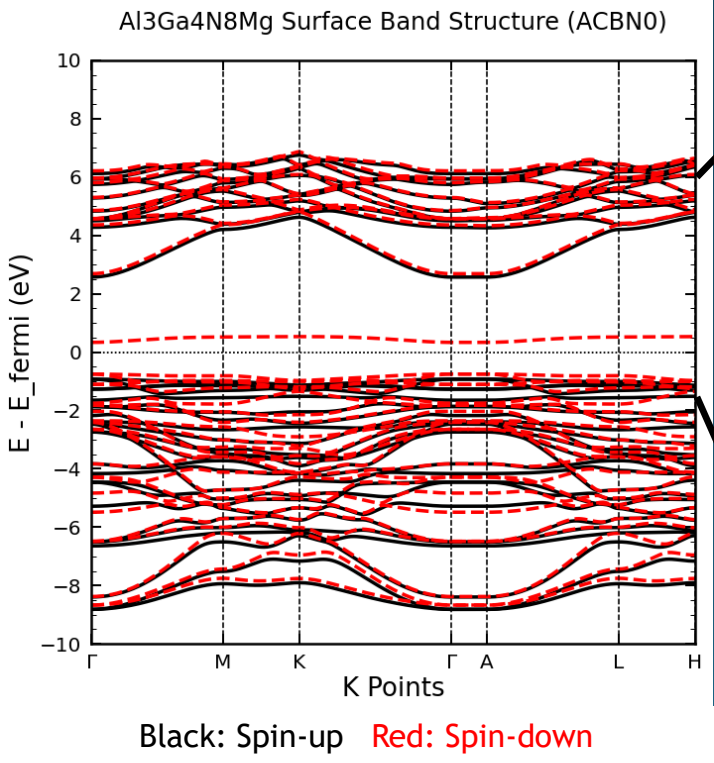
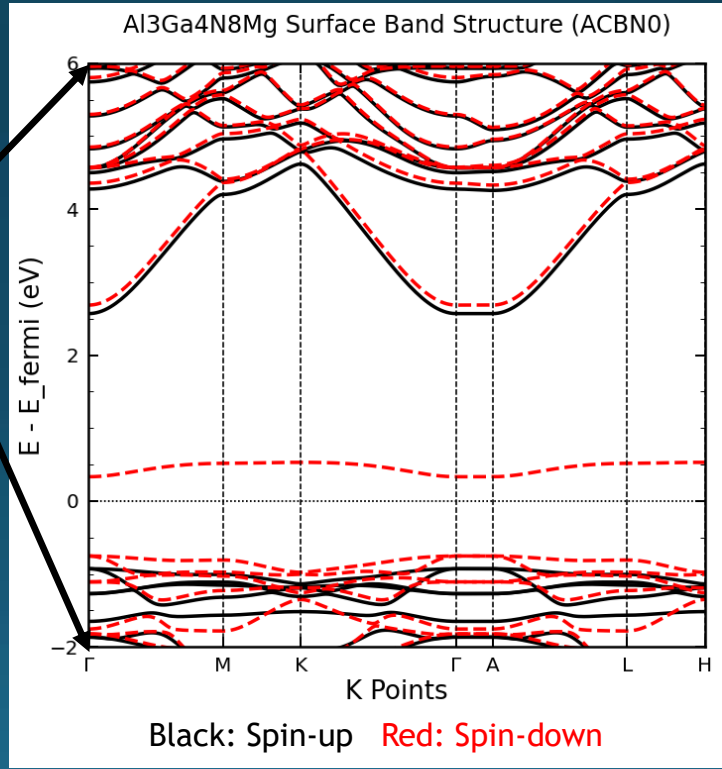
p-Doped Monolayers







Results:

- Alloy formation is exothermic.
- Magnetization is -1 Bohr magneton, as expected.
- Spin-polarized top of valence band.

➔ Insulator.

➔ Isolated State in gap.

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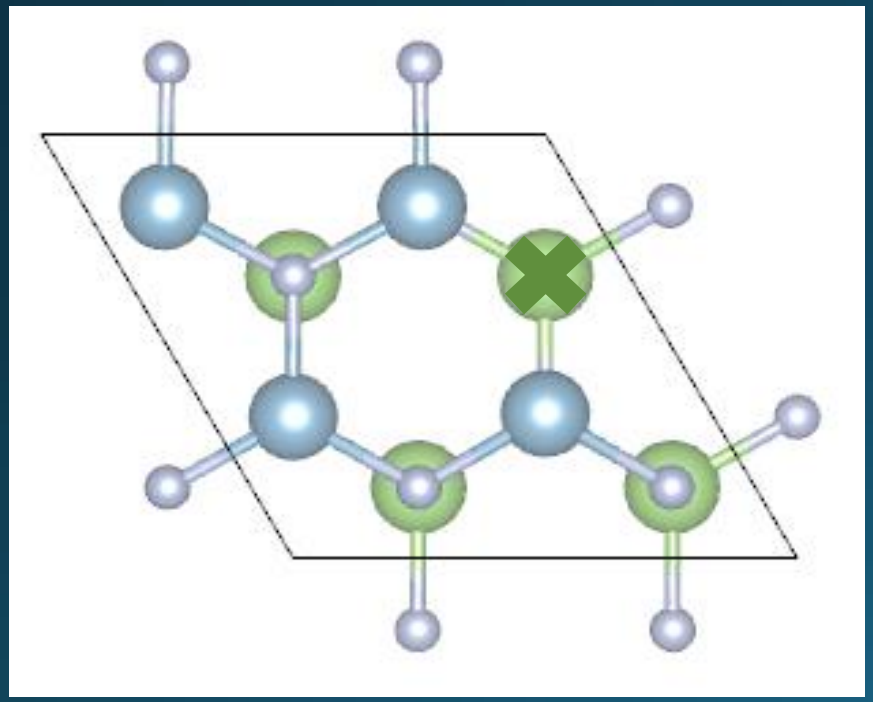
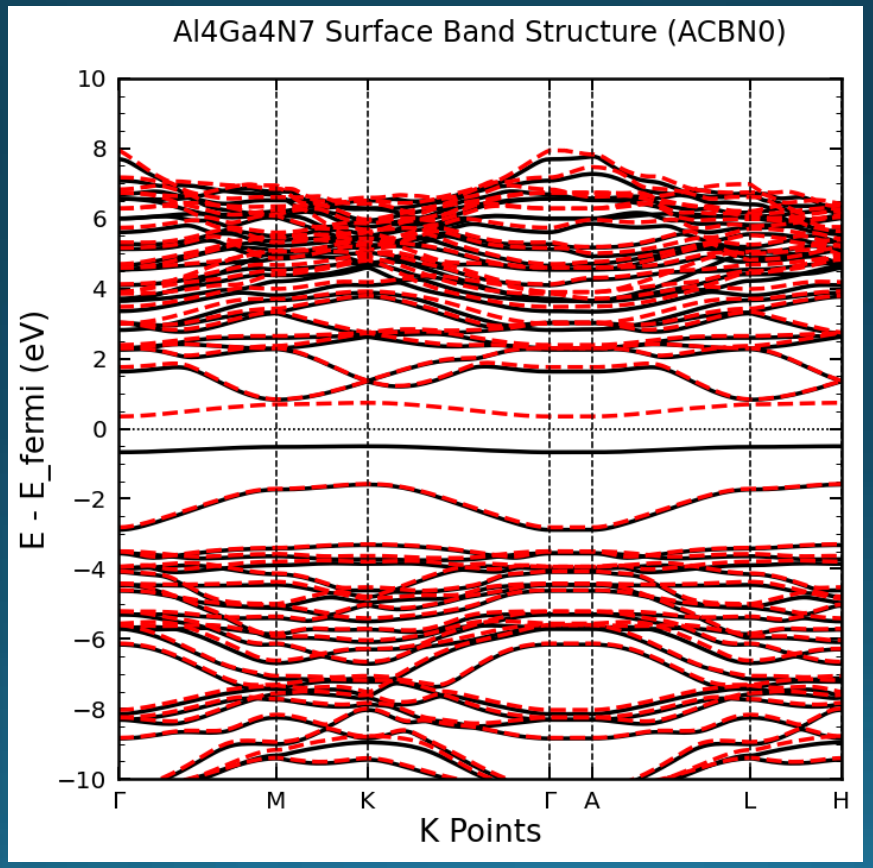
Vacancies in Monolayers





Results:

- Isolated (occupied) defect state.
- Low dispersion (unoccupied) defect state.
- Spin-polarized.

➔Spin-1/2 qubits?
➔ Spintronics?

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Impact of Work

- Improved computational treatment of AlGaN system, ACBN0.

- Mg and Si dopants likely condense at or near surface, interfaces, and other defects.
- Bulk doping is unlikely.

- Asymmetric surface/interface: metal and nitrogen truncation.
- Surface/interface are predicted to be metallic $\Leftrightarrow$ $E_g = 0$ eV.

➔ Interface formation could explain the reduced diode performance observed by the LDRD team.

- Monolayer vacancy may realize compact spin-1/2 qubit.

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Challenges and Risks / Next Steps and Future Work

Challenges and Risks

- None.

Next Steps

- Thermochemistry of AlGaN surface in the presence of Mg, Si dopants.
- Build interface and verify:
  - Mg, Si dopant accumulation.
  - Verify that our current conjecture that p-GaN//graphene//p-AlGaN interfaces are metallic and cause LDRD observed diode performance degradation.

Monolayer AlGaN

- Spin-1/2 qubits? Spintronics?