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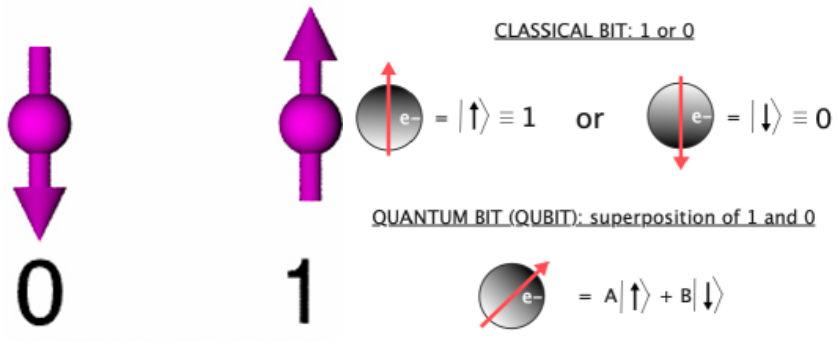
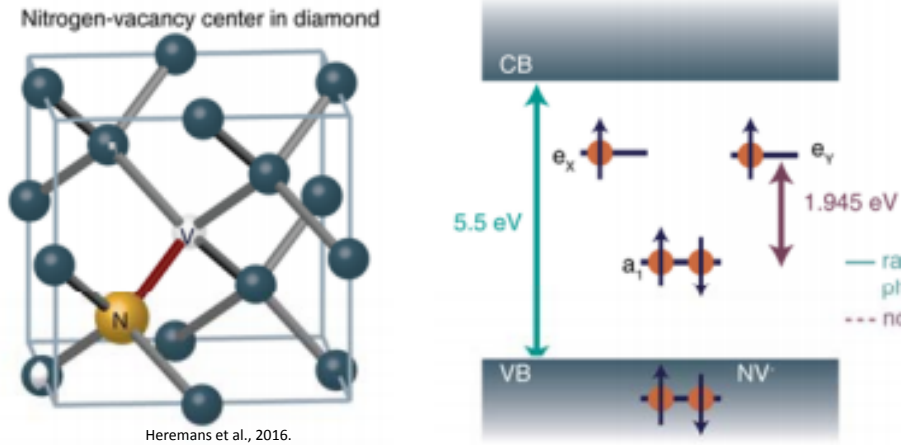
Engineering Defects in AlGaN for Advanced Information Processing

Authors: Jeremy Kamin (PhD student in Physics), Dr. Boris Kiefer (New Mexico State University), Dept of Physics, Dr. Julia Deitz (Sandia)

Introduction and Motivation





Heremans et al., 2016.

- **Qubit – superposition of two quantum states for quantum computing and quantum sensing:**
  - Electron spin is ideal candidate.
- **Currently, Nitrogen-vacancy center in diamond is a good candidate for creating qubits:**
  - Isolated electronic states inside the band gap. (Seo et al., 2016)
  - Challenge: Diamond is costly and difficult to manipulate.
- **LDRD material set: AlN, GaN, and AlGaN:**
  - Large bandgap: $E_g > 3$ eV
  - Electron and hole doping.

Objective: Create new material platform for advanced information processing and sensing.

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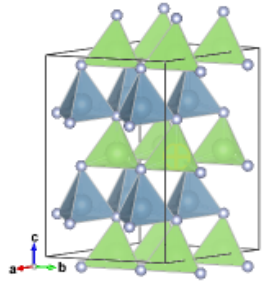
Computational Approach

- Quantum Espresso (Giannozzi et al., 2017)
  - Use Density-Functional-Theory (DFT) to compute defect related electronic states.
  - Ecut == 70 Ry; Kpoints >= 3 x 3 x 2
  - Generalize-Gradient-Approximation (PBE, Perdew et al., 1996)

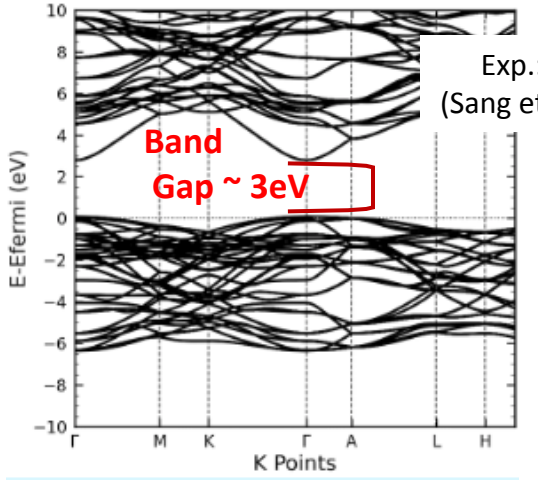
Challenge:
DFT systematically underestimates band gaps.

Improvement:
- ACBN0 (Agapito et al., 2015).

Known Crystal Structure:
- **Hexagonal (equilibrium phase).**
- **Ferroelectric.**
- **Corner sharing tetrahedral network.**

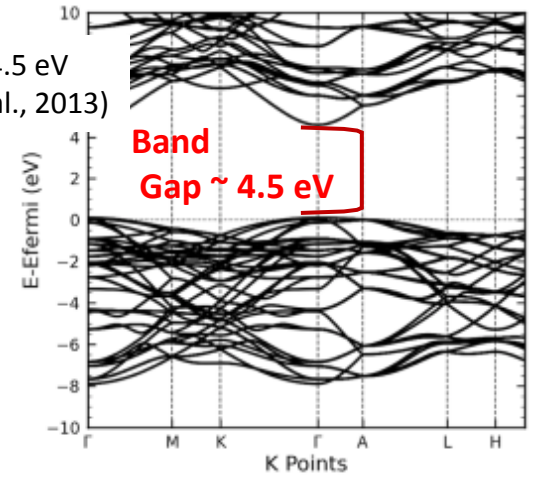


DFT AlGaN Bands



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

ACBN0 AlGaN Bands



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Data Science – Dopant Selection

Intro

Dopant selection:

- Matching ionic radii.
- Eliminate energy dissipation pathways: dominant nuclear S=0 isotope; low spin-orbit coupling (Weber et al., 2010).

Analysis

Host Material AlGaN:

- GaN S-O constant = 137 cm^{-1}, AlN S-O constant = 153 cm^{-1}, comparatively low values.
- Investigate (known) element/property correlations across the periodic table.

Element	Charge	Coordination	Ion Radius
Al	3	4	0.39
		5	0.48
		6	0.535
Ga	3	4	0.47
		5	0.55
		6	0.62

Elements	Z/A	Spin Orbit Coupling Constant (cm-1)	Natural Abundance (%)
Radii Diff <=.12			
Chromium	24/52	248	83.789
Nickel	28/58	691	68.27
Iron	26/56	431	91.72
Titanium	22/48	123	73.8
Tin	50/120	1855	32.59
	50/118		24.22
Magnesium	12/24.	40.5	78.99
Radii Diff <= .20			
Zinc	30/64	390	48.6
	30/66		27.9
Platinum	78/194	4481	32.9
	78/196		25.3
Zirconium	40/90	387	51.45
Silicon	14/28	130	92.23

Insight

Most promising elements: Si, Cr, Ti, Mg, and Fe.
Here we report on Si and Cr dopants.

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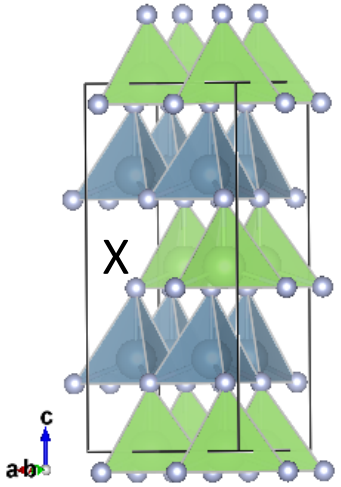
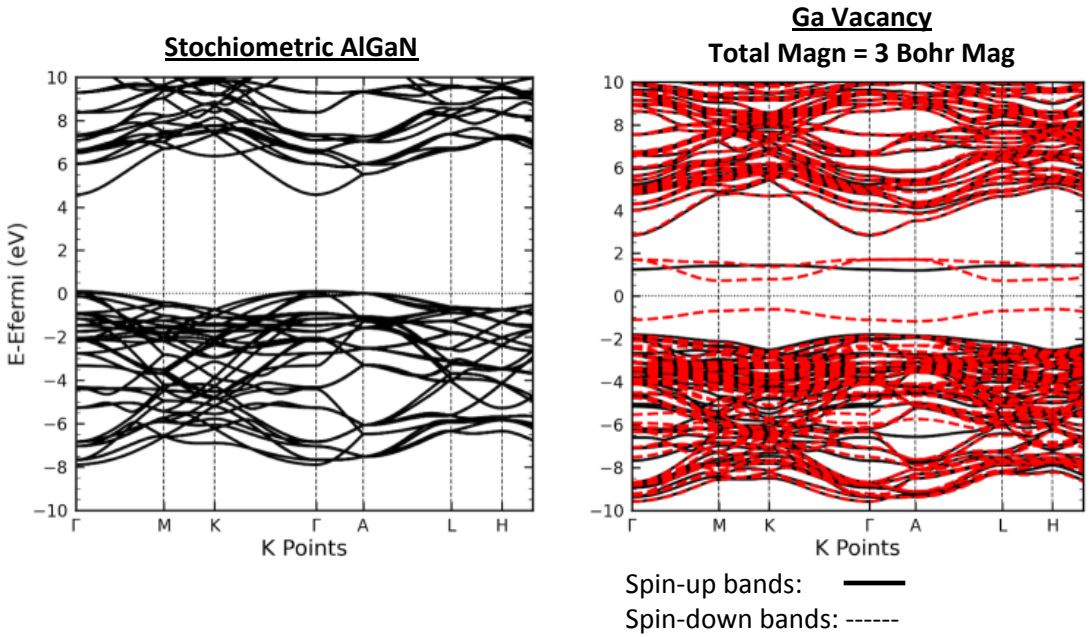
Ga Vacancy in AlGaN





Explanation: m=3 μ_B.
Ga vacancy formation
➔ Three dangling electrons.
➔ High-spin arrangement. All spins are aligned.

Insight

- Spin polarized isolated states in band gap.
- Dispersion => likely delocalized states; quantum entanglement?

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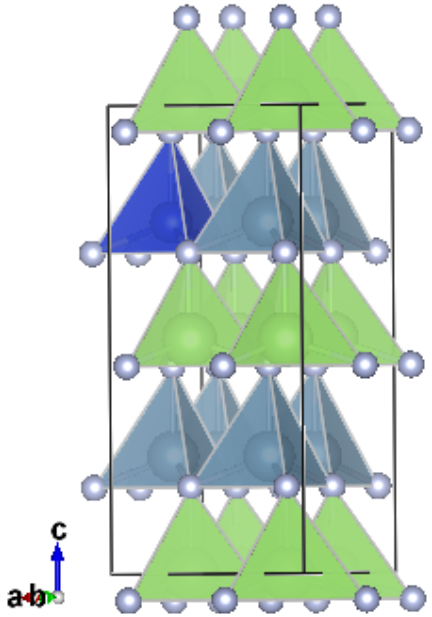
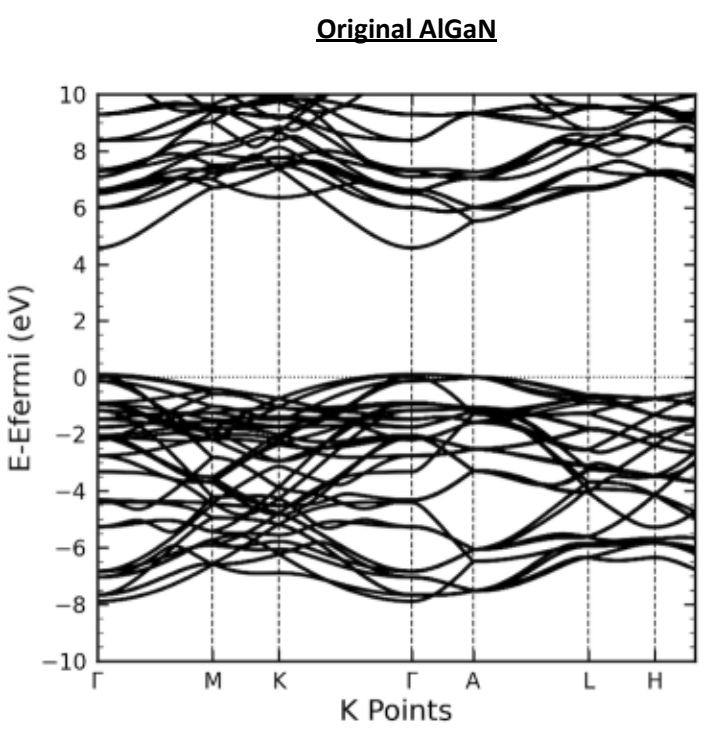
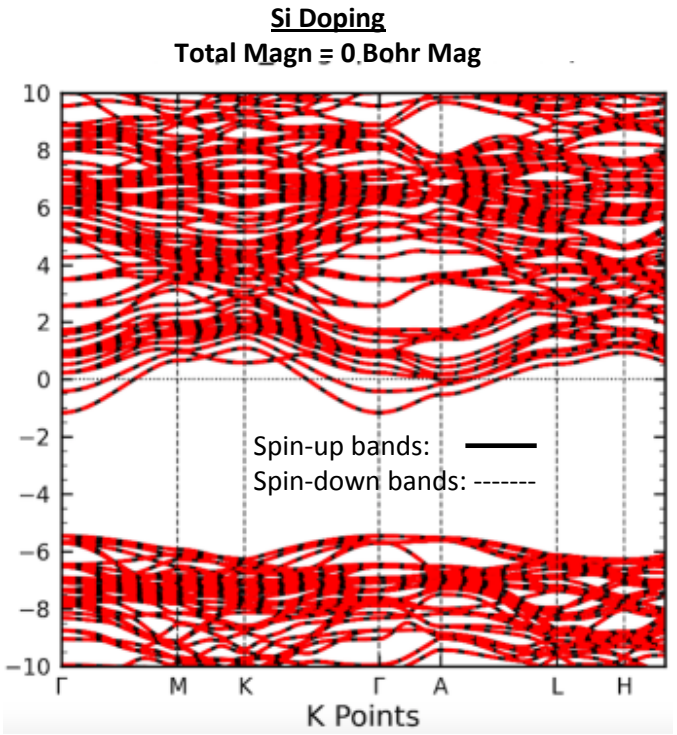
Si Doping in AlGaN







Explanation:

Si doping: electron donor, only states available are close to conduction band => Fermi energy moves into the conduction band.

Insight

- Si doping: new states at bottom of conduction band. Infrared sensing?

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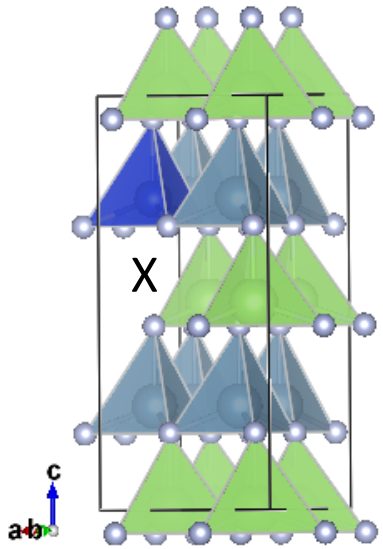
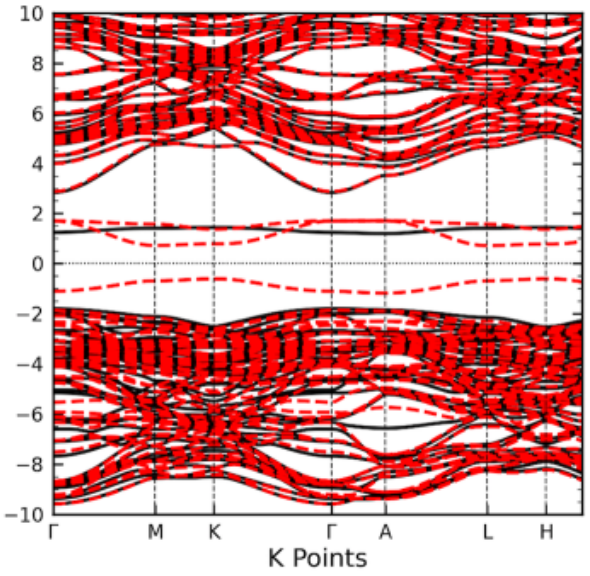
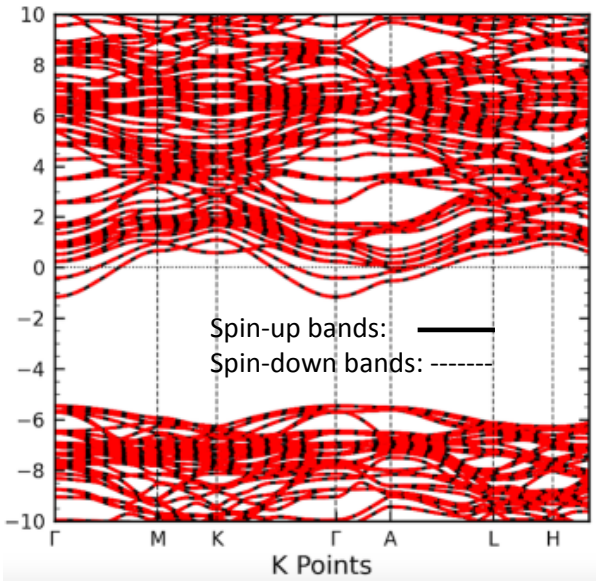
Ga Vacancy and Si Doping in AlGaN



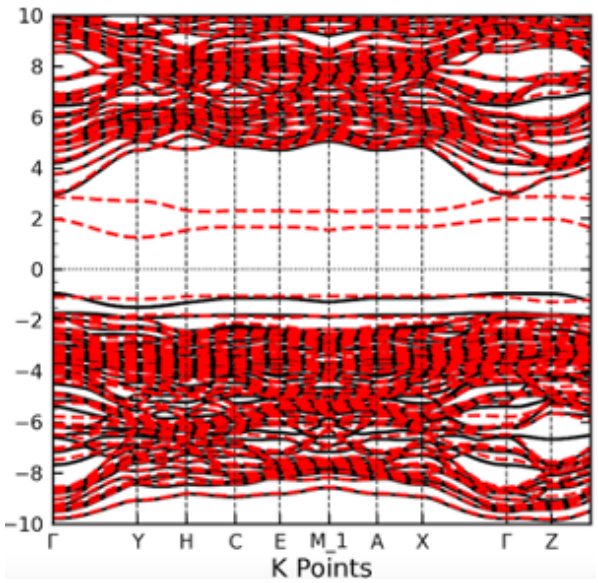
Ga Vacancy
Total Magn = 3 Bohr Mag



Si Doping
Total Magn = 0 Bohr Mag



Ga Vacancy + Si Doping
Total Magn = 2 Bohr Mag



Insight

- Ga vacancy + Si dopant: spin-pairing ➔ antiferromagnetic system Spintronics?
- Unoccupied states spin-polarized >~ 3eV higher in energy, likely inferior to diamond N-V defect.

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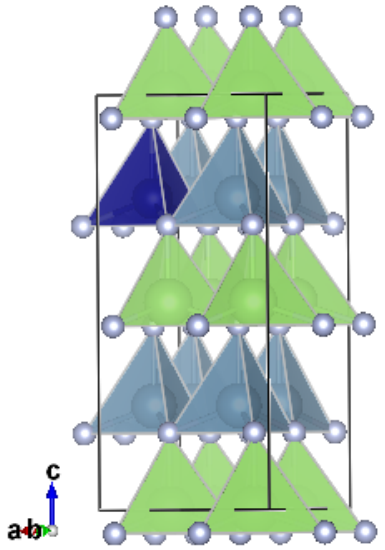
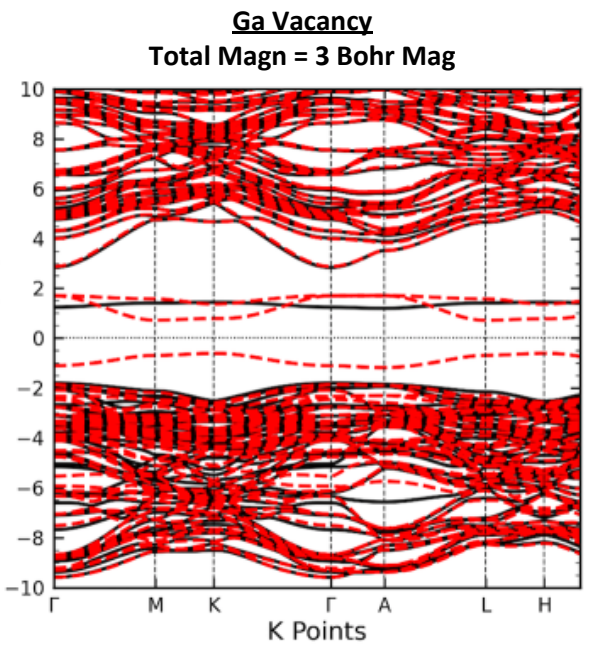
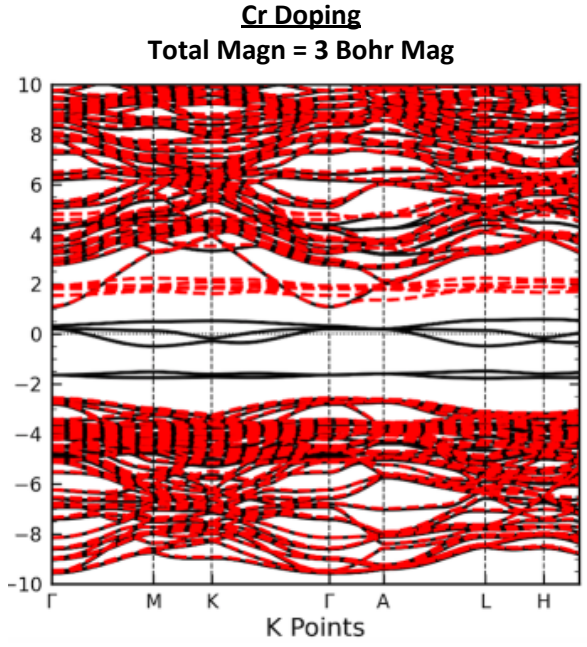
Cr Doping in AlGaN







Spin-up bands: ——

Spin-down bands: -------

Explanation

Cr: $4s^1 3d^5$

3 electrons to host crystal, three electrons remain.

Unpaired => m = 3 μ_B.

Insight

- Cr doping: spin polarized at Fermi level. Spin qubit? Spin filter? Spintronics? .

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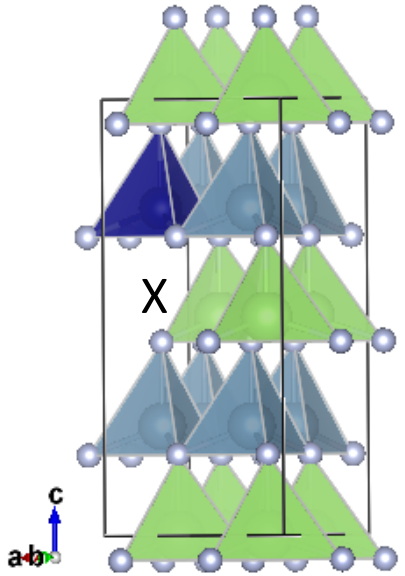
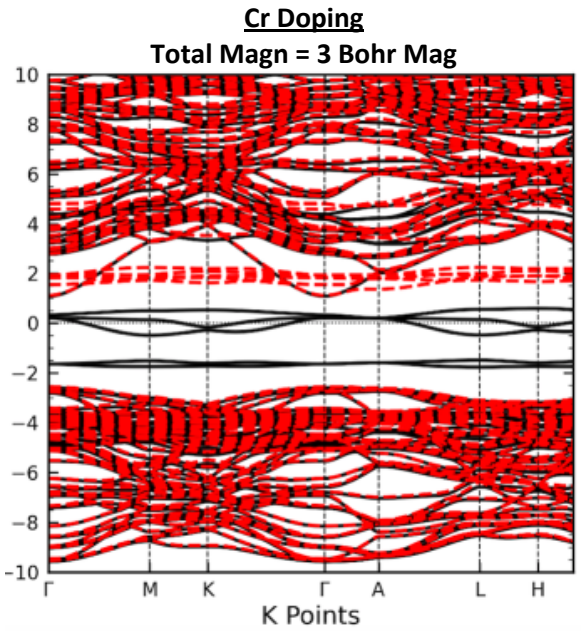
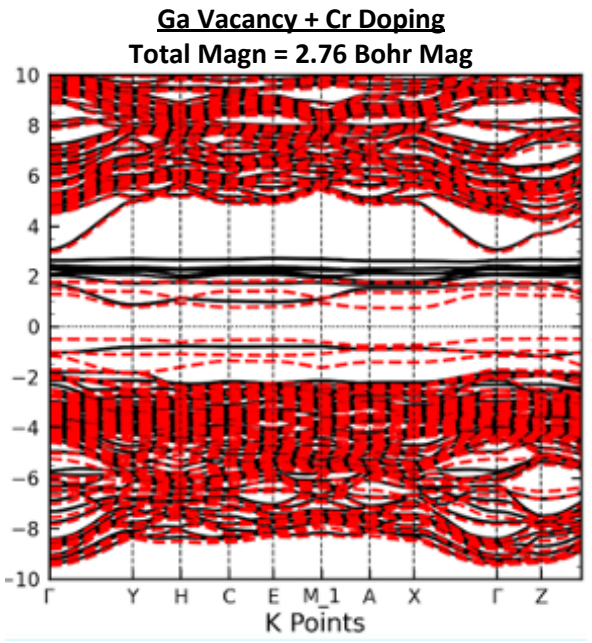
Ga Vacancy and Cr Doping in AlGaN







Spin-up bands: ——

Spin-down bands: -------

Observation:

3 extra Cr electrons create a complicated spin-polarized occupied and unoccupied states.

Insight

- High number of excess electrons: Dopant + vacancy => complicated electronic structure, overlapping spin -up and spin-down states => likely unsuitable for qubit design, but may be suitable for information storage, spintronics.

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Impact of Work

- Vacancies and doping + vacancies create isolated defect states in band gap of host material.
- Computed defect states allow for establish defect/technology correlations:

  Ga vacancy: spin qubit?

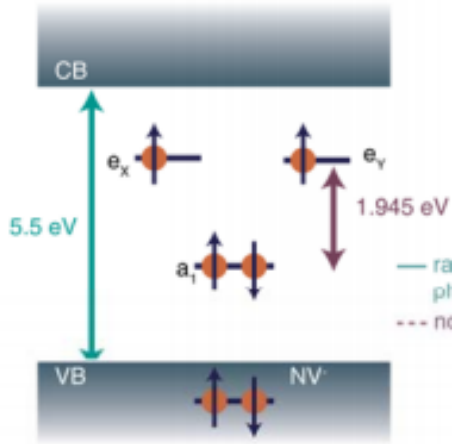
  Si_{Al} doping: infrared sensing?

  Si_{Al} + Ga vacancy: robust spintronics?

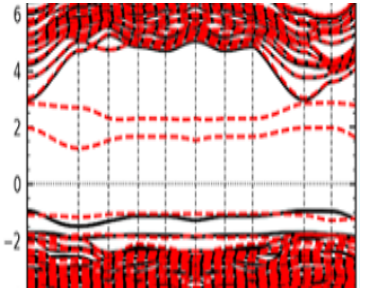
  Cr_{Al} doping: spintronics?

  Cr_{Al} + Ga vacancy: spintronics.

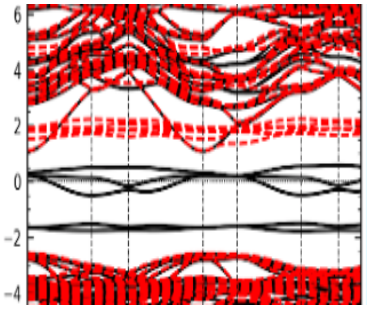
- Recommended design principle for AlGaN spin qubits: Minimum deviations from host: +2 (hole) and +4 (donor) ions.



Ga Vacancy + Si Doping



Cr Doping



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Challenges and Risks / Next Steps and Future Work

- Challenges and Risks:

  None

- Next Steps/Future work:
  - Rehybridization due to spin-orbit coupling.
  - Following our learned design principle, test Ti, Mg, Fe.
  - Evaluate thermodynamics of alloy formation.

Evaluate electronic defect states for advancing spin-based technologies:

Quantum computing, quantum sensing, spintronics.

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Nickel	28/58	691	68.27
Iron	26/56	431	91.72
Titanium	22/48	123	73.8
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