Understanding radiation-induced lattice defects in $Al_xGa_{1-x}N$ systems

Mia Jin, Farshid Reza, Alex Hack, Mahjabin Mahfuz, Xing Wang, Blair Tuttle

mmjin@psu.edu

Penn State University

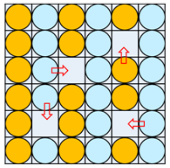
FY2024: we delve into the defects in $Al_xGa_{1-x}N$

Poster by Farshid Reza:

Exploring Al/GaN Defects with Molecular Dynamics

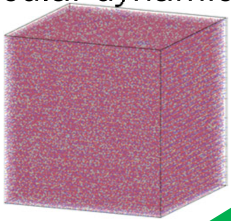
- ❖ Electronic effects
- ❖ Radiation-induced defects

- Kinetic Monte Carlo



- ❖ Electronic effects
- ❖ Defect properties
- ❖ Carrier capture cross-section

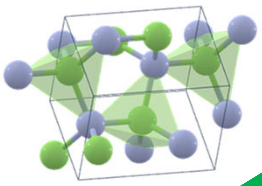
- Molecular dynamics



Poster by Alexander Hauck:

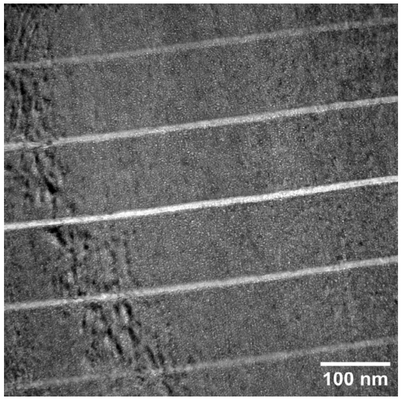
First-principles calculations of nonradiative carrier capture for defect complexes in AlGaN systems

- Density functional theory



Time & Lenth

TEM image showing Al dependent defect formation by 950 MeV Au ion irradiation



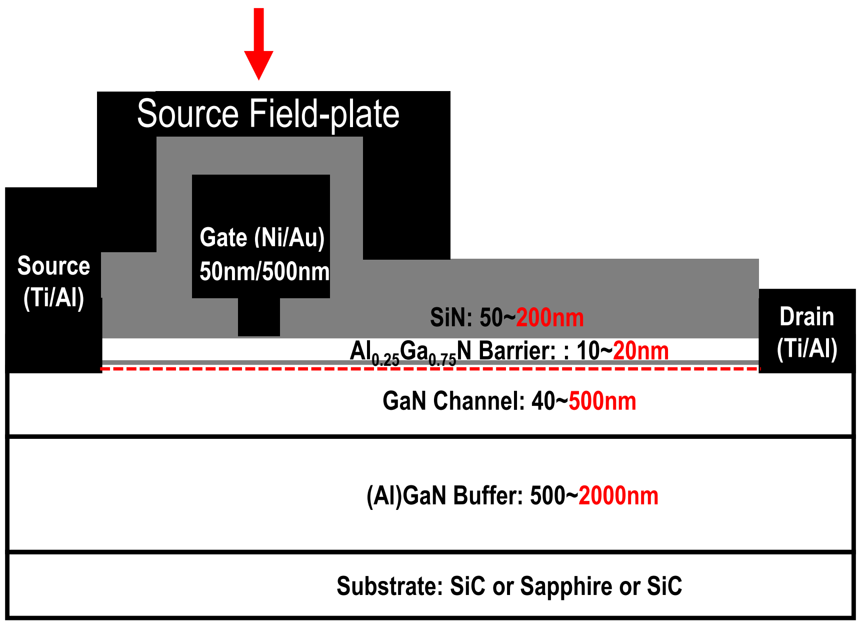
Poster by Mahjabin Mahfuz:

Transmission Electron Microscopy and Atomic Probe Tomography Characterization of Swift Heavy Ion-Induced Cavities in GaN

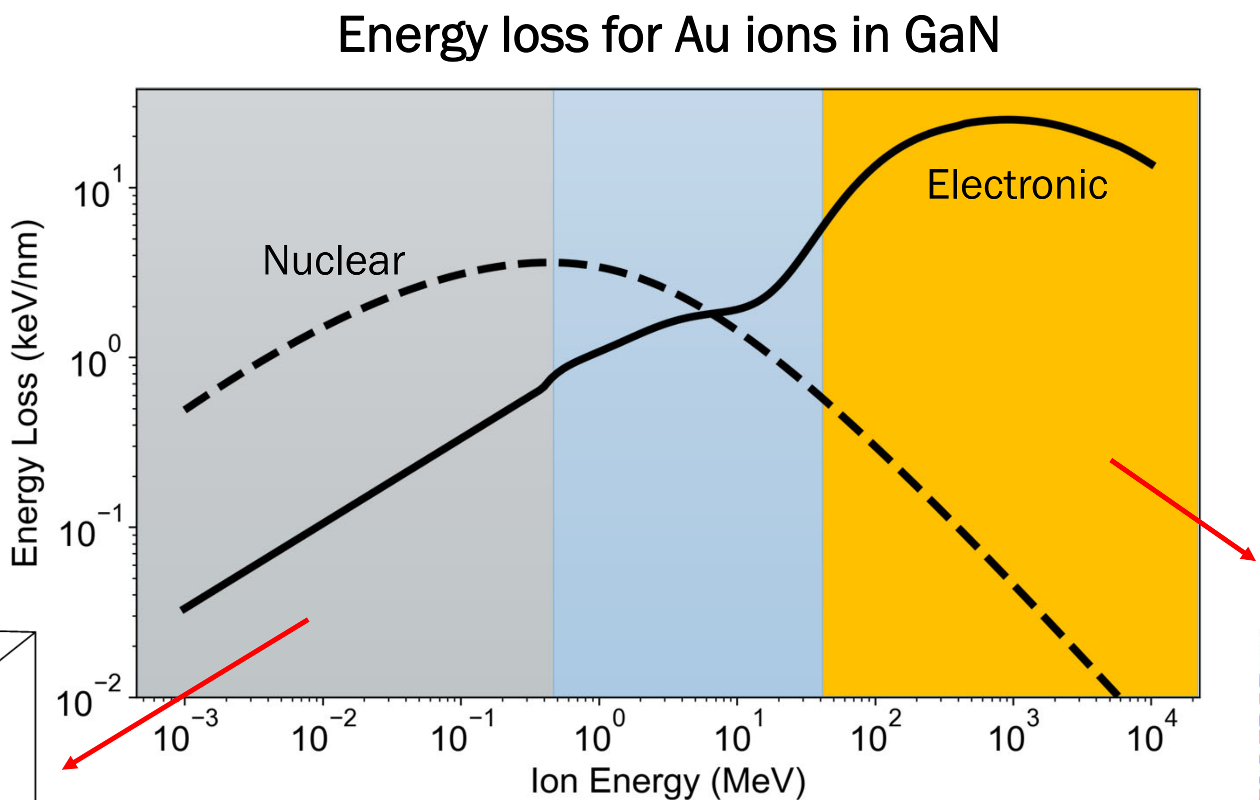
HEMT GaN device under irradiation

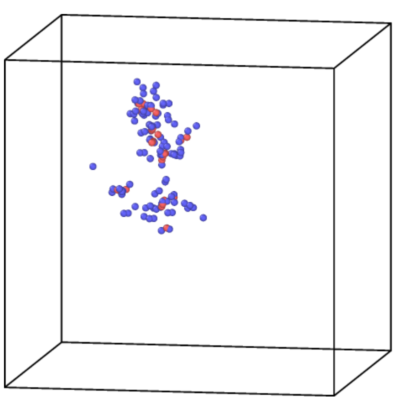
To reflect the space radiation environment, two radiation conditions are considered:

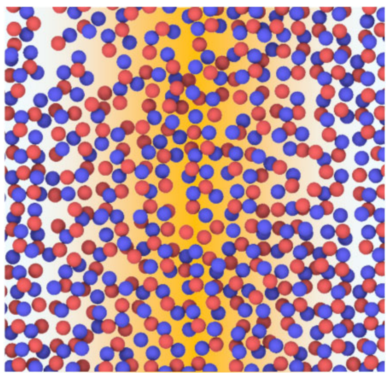
- Swift heavy ion (SHI) irradiation: single events effects
- MeV level ion irradiation: accumulated damage effects



Ion energy-dependent energy loss





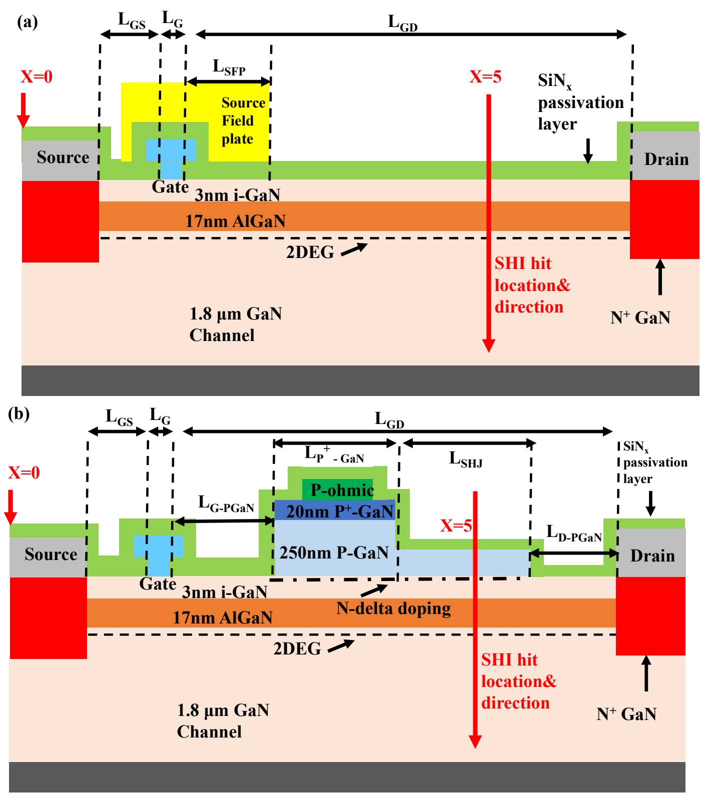


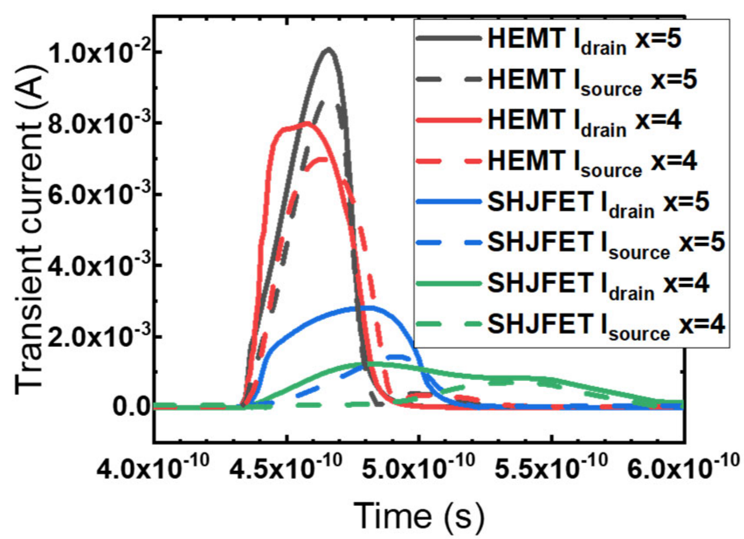
SHI induced single event in devices

- HEMT: Single event transient current due to the punch-through effect by local increase of electrostatic potential.
- SHJEFET: Improved E-field management and a more favorable potential profile to suppress transient current peak.

HEMT

SHJFET



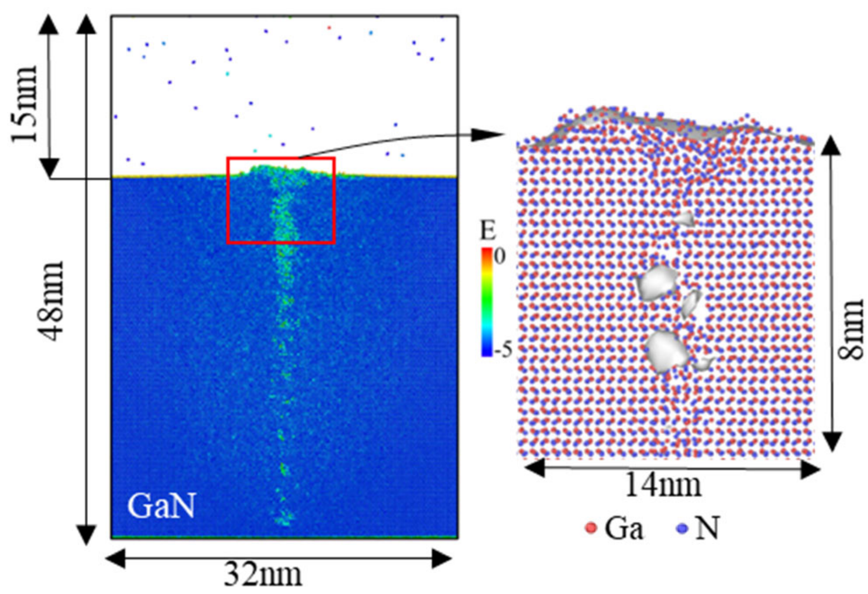


Song, et al. "Physics-based 3D simulation of single event transient current in GaN high-electron-mobility transistor and super-heterojunction field-effect transistor." *Applied Physics Letters* 124.17 (2024).

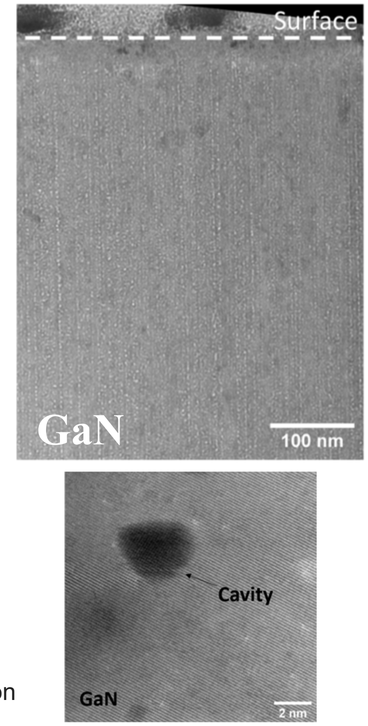
Structural changes due to SHI

- 950 MeV Au ions in GaN (44.5keV/nm, LET: 72.36MeV·cm^2/mg) induce cavities along the track.
- Minimal amorphization even at very high fluences (8x10^{12} /cm2).

Molecular dynamics simulations



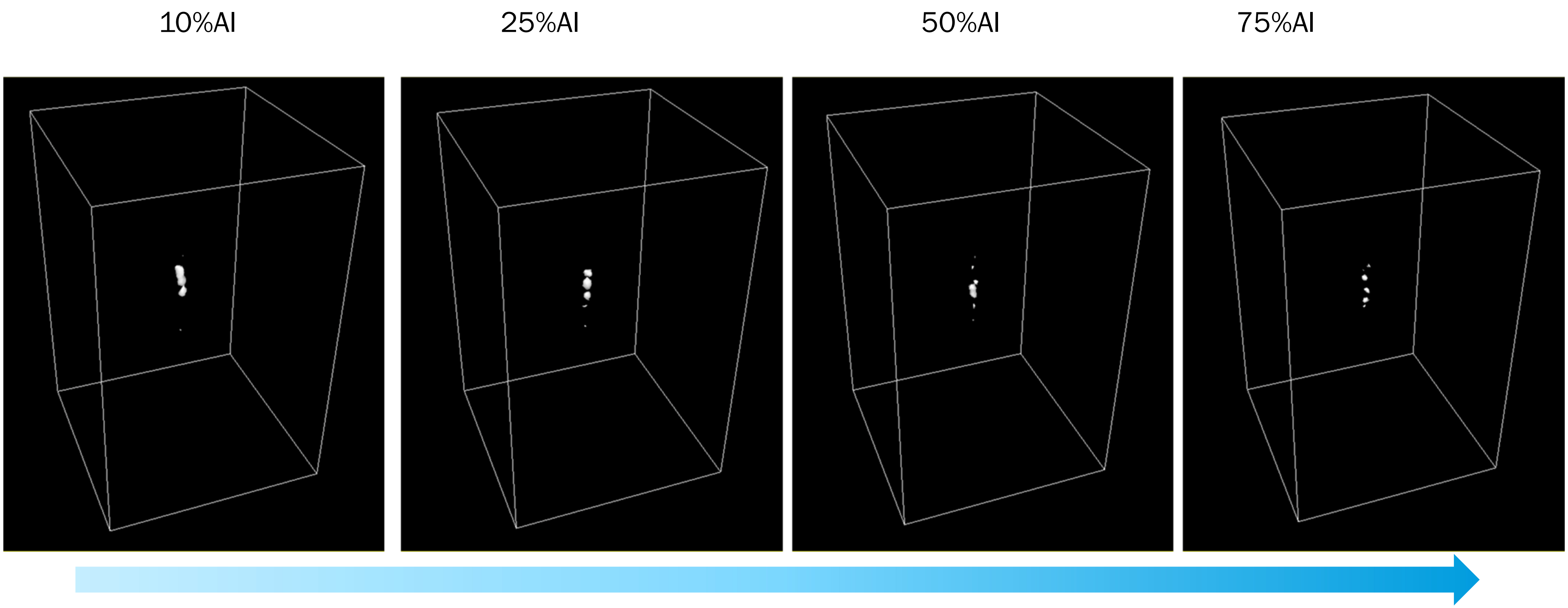
Transmission electron microscopy



Mahfuz, et al. "Microstructural changes in GaN and AlN under 950 MeV Au swift heavy ion irradiation." *Applied Physics Letters* 124.11 (2024).

Al-content dependent cavity formation

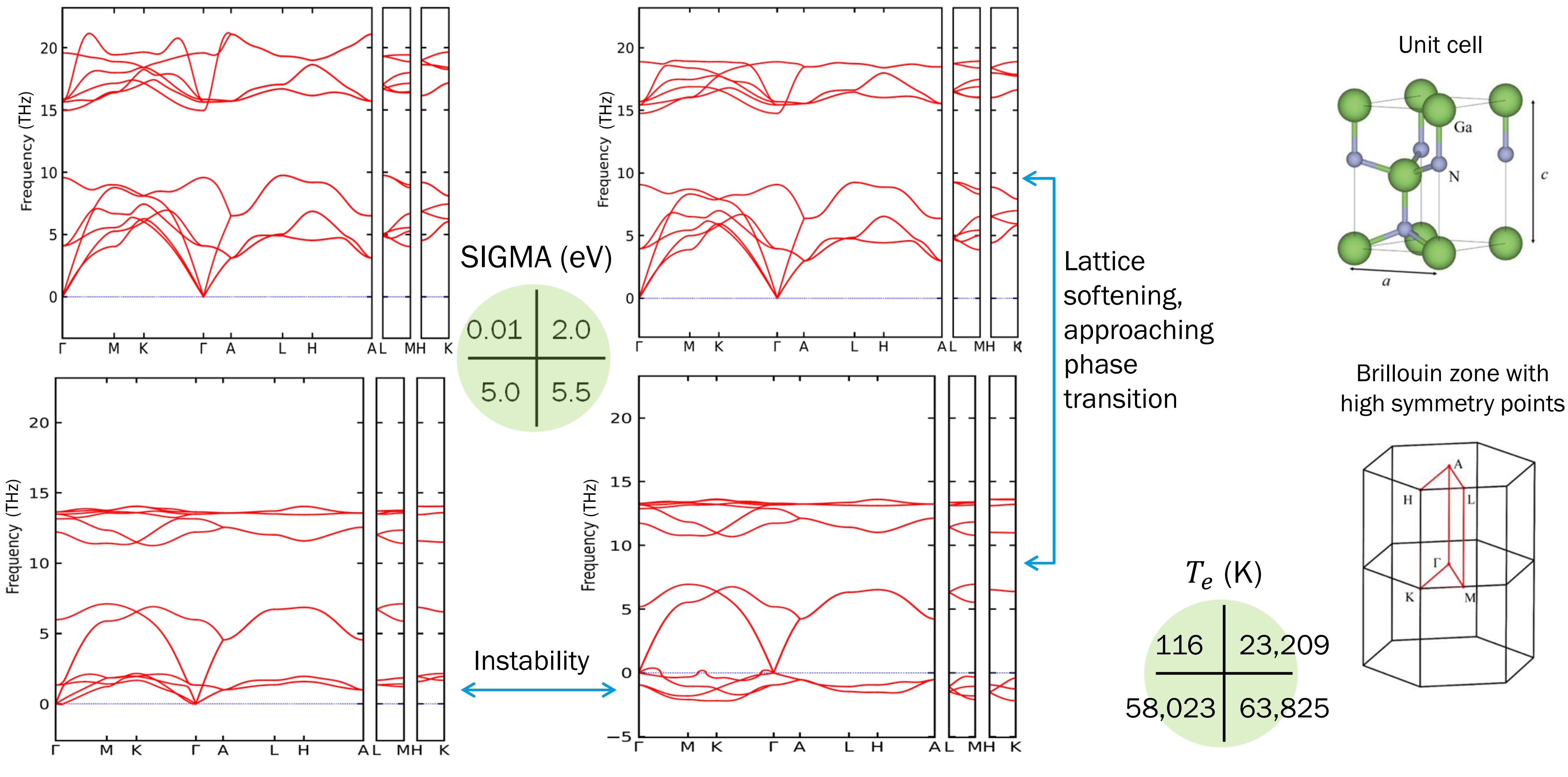
- MD simulations predict experiment-consistent trends (Dr. Wang's talk).



With increasing Al concentration, less likely to form cavities.

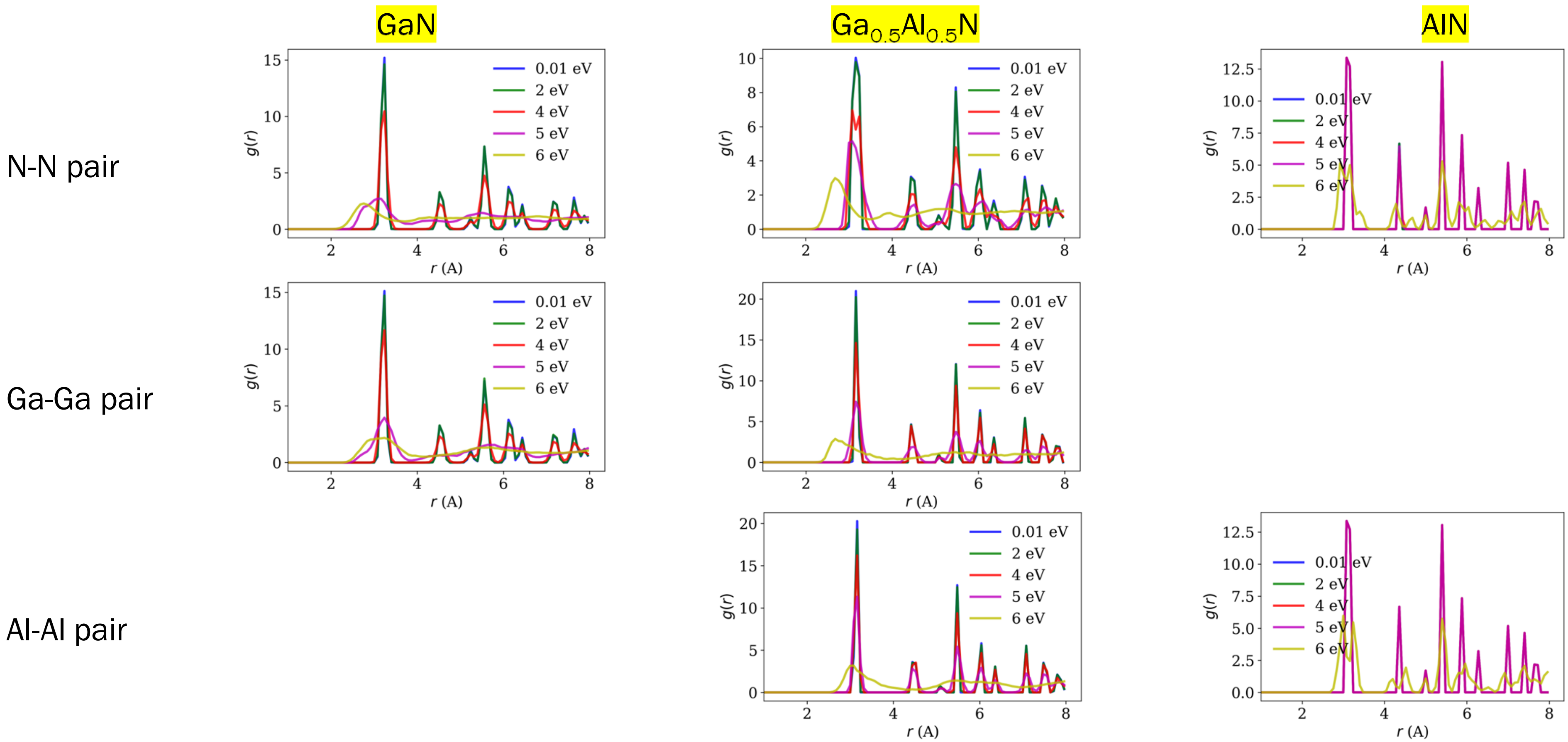
First-principles understanding of lattice instability

- Varying the electron temperature: phonon dispersion in GaN



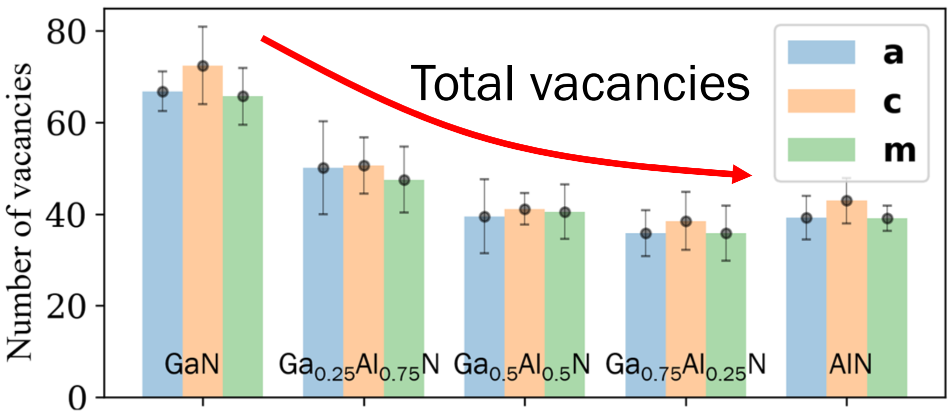
Effect of electron temperature

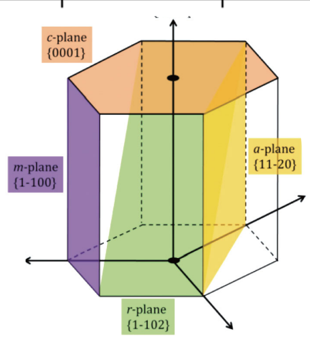
- Al-content dependent dynamics: increasing Al content enhances lattice stability.
- N sublattice appears to break first.

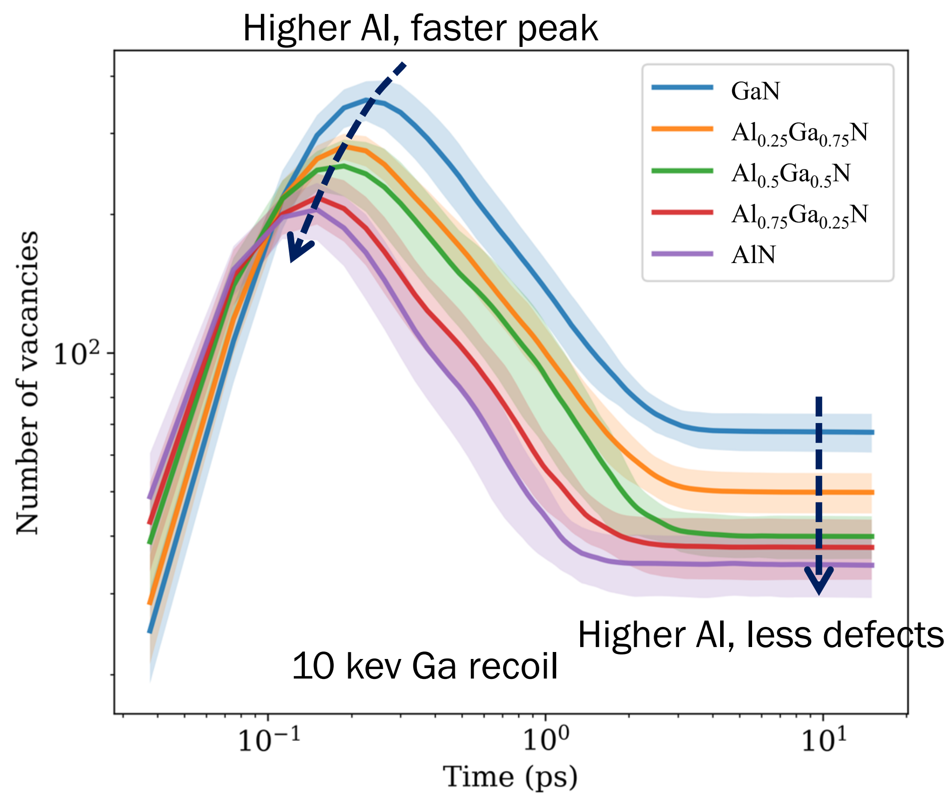


MeV-level ion radiation response

- Primary radiation damage simulations of energetic recoils.
- Residual defects from 10 KeV Ga at 300K: Similar in defect production along different crystalline directions; Strong dependence on Al-content.

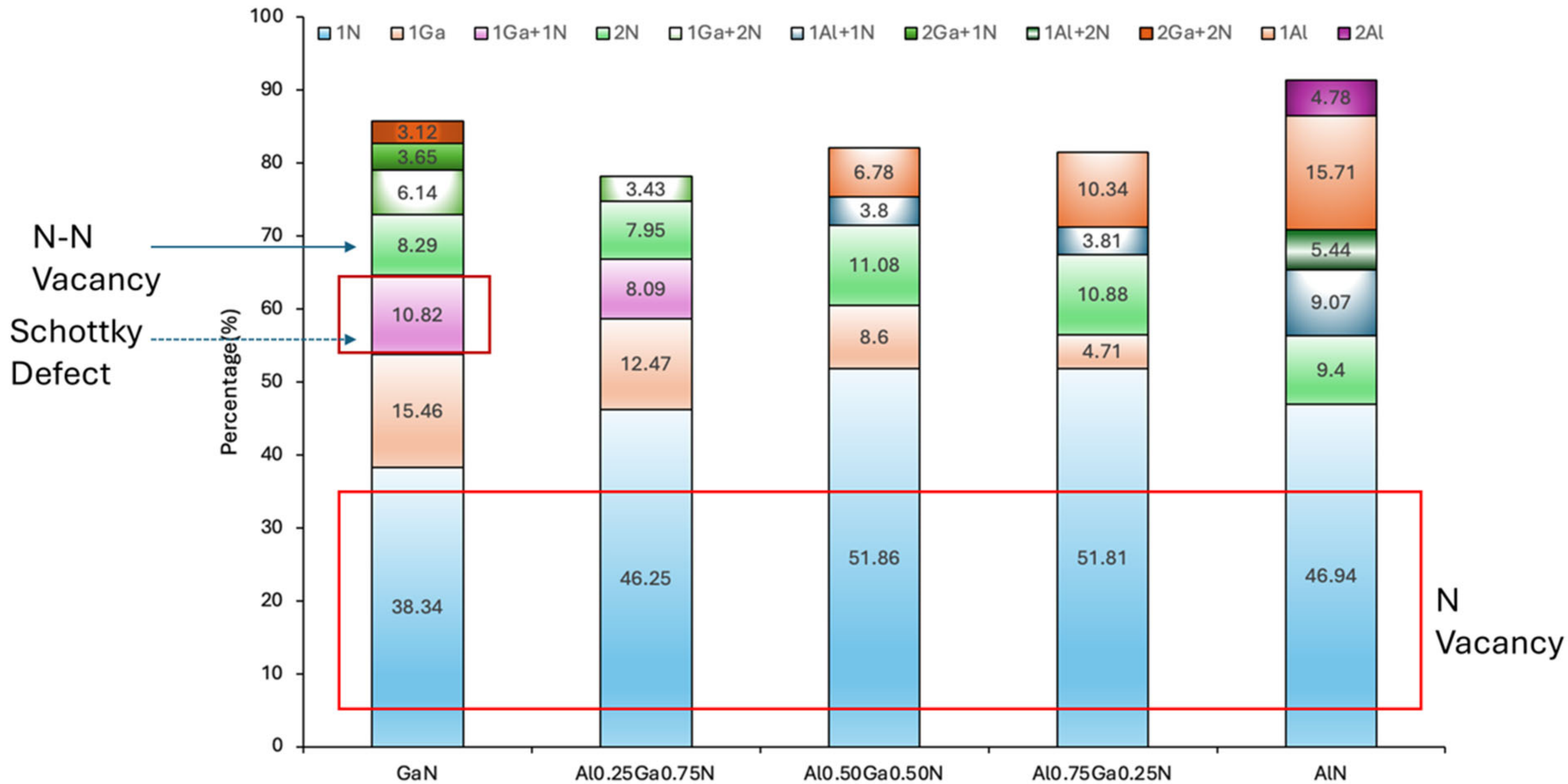






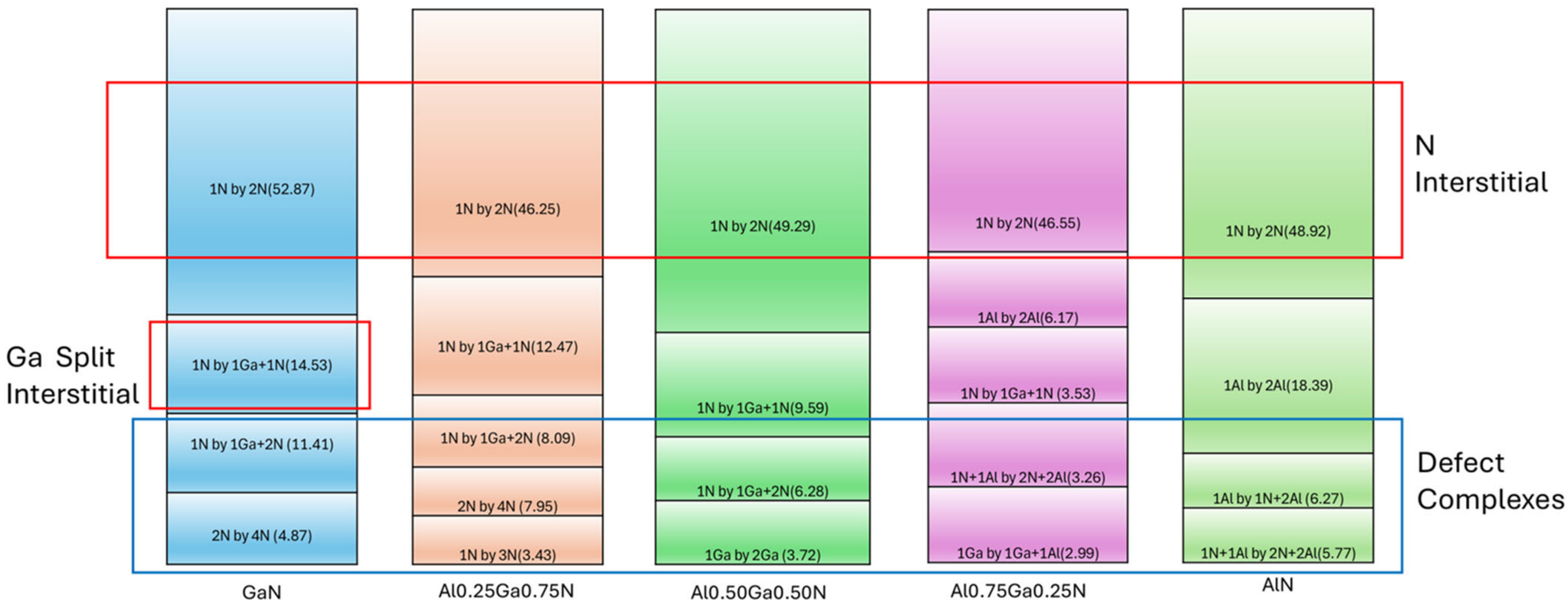
Vacancy defects & clusters

- Majority of the defects are nitrogen vacancies
- Notable vacancy clusters: N-N, Ga-N.



Interstitial defects & clusters

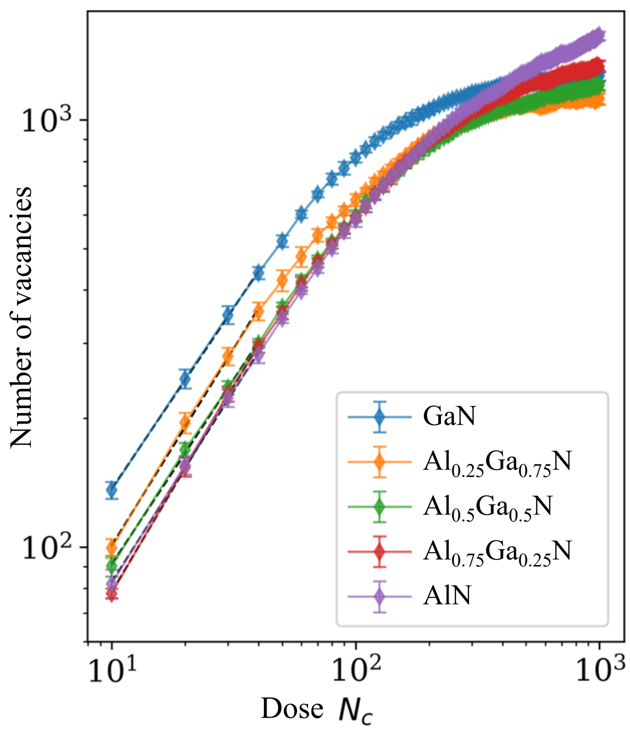
- More than half are N interstitials (octahedral site with formation energy of 4.14eV in N-rich condition)

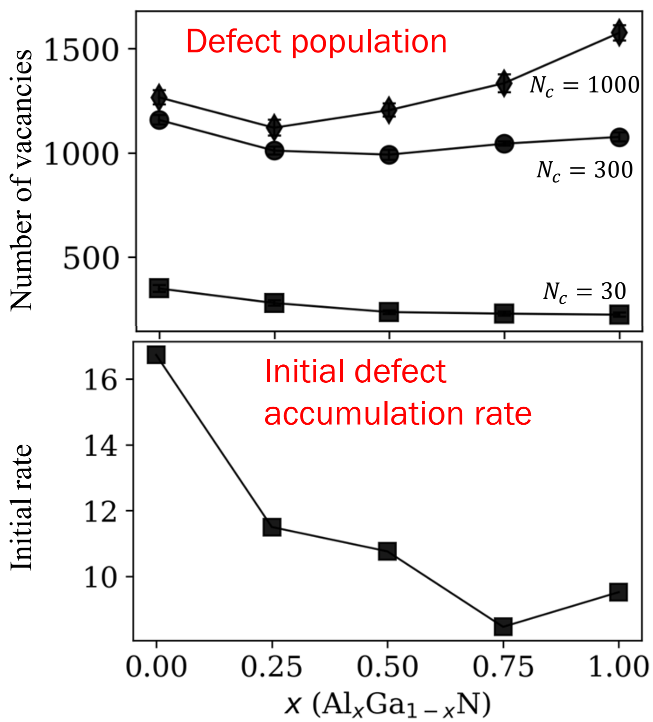


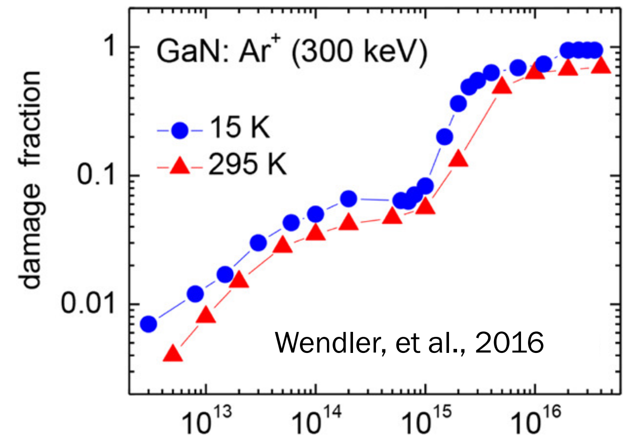
Note: height not to scale, percentage in parathesis

Extended radiation response

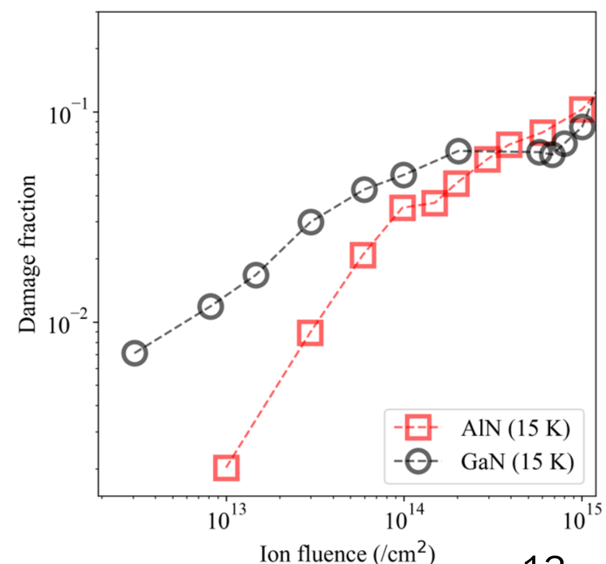
- GaN highest defect accumulation rate
- AlN highest damage at high dose
- Optimal Al fraction exists





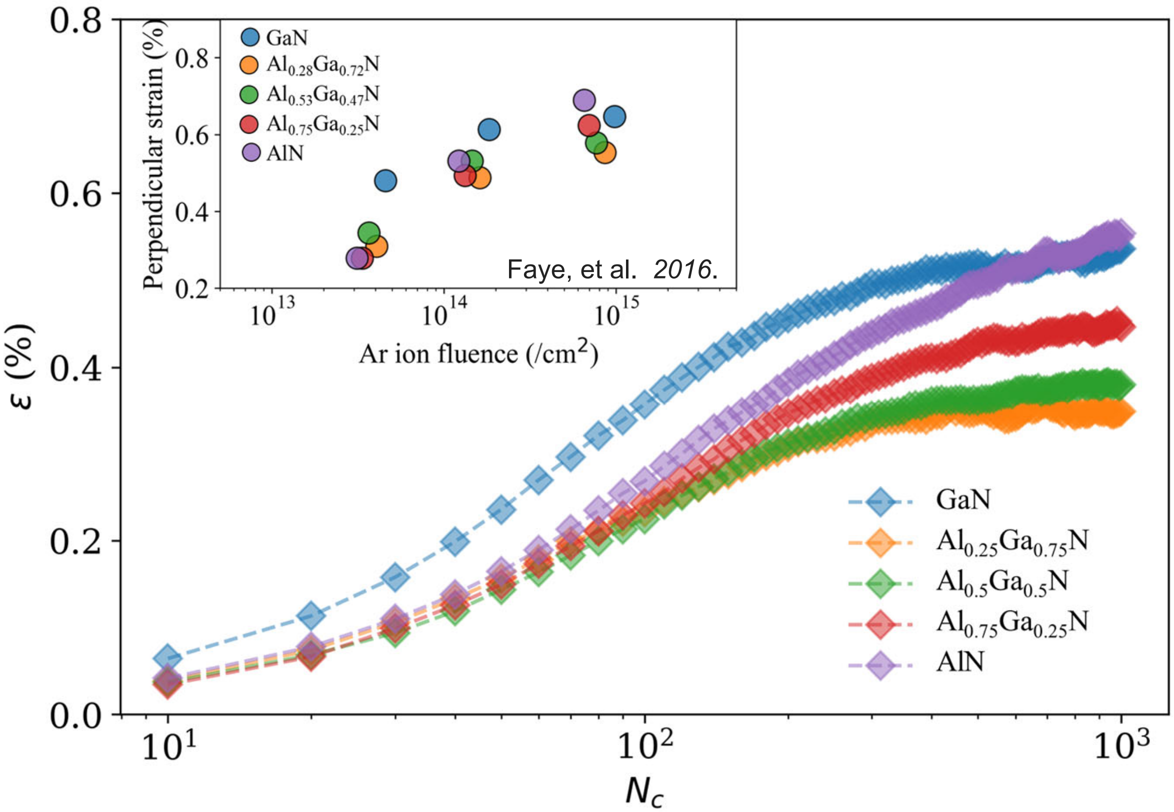


Experimental measurements



Radiation-induced strain

- Highly consistent with experimental measurements.
- MD simulations nicely capture the radiation phenomena before phase transition. Difference in responses is attributed to extended defects formation.



Enhancement with AI

- Defect energetics based on machine learning interatomic potentials.
- Working on publication for potential assessment.

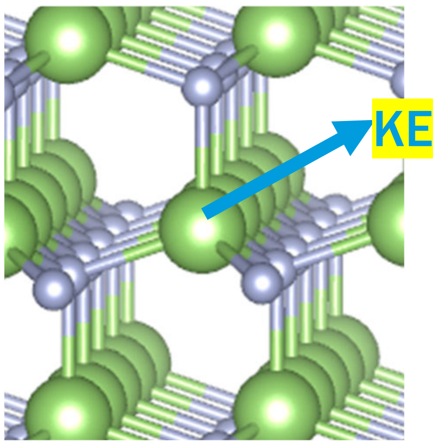
Defect Formation Energy (eV)

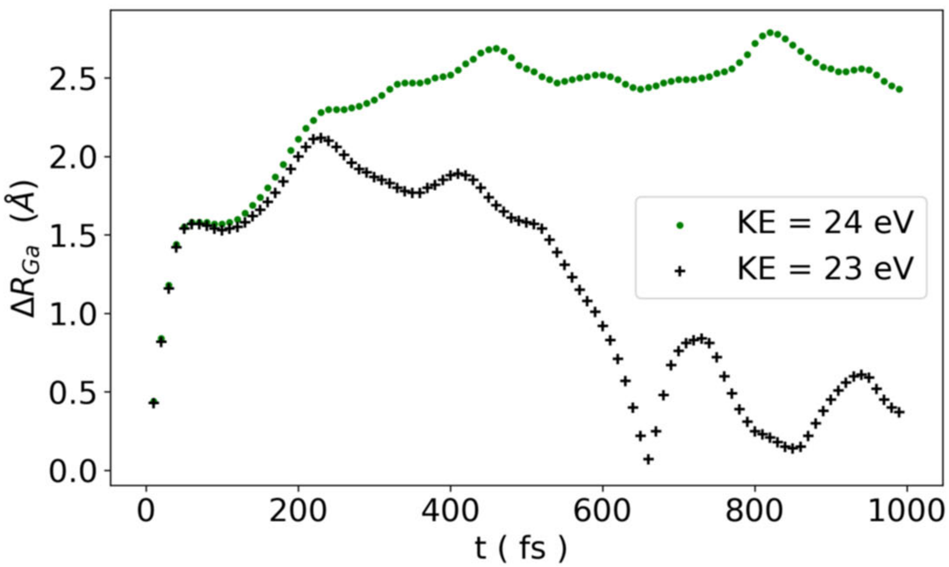
Defect type	AlGaN ML potential	GaN ML potential	AlN ML Potential	*Lei et al. (DFT)*	*Zhu et al. (Interatomic Potential)*	
					2body	*3body*
$V_{Ga\text{-}N}$ in GaN	6.42	4.92		6.66		
Ga_{FP} in GaN	10.09	8.36		10.07		
N_{FP} in GaN	7.31	8.59		7.32		
Al_{FP} in AlN	10.44		16.79		9.74	10.47
N_{FP} in AlN	9.25		9.35		9.73	10.52
$V_{Al\text{-}N}$ in AlN	6.06		7.25		7.63	8.16

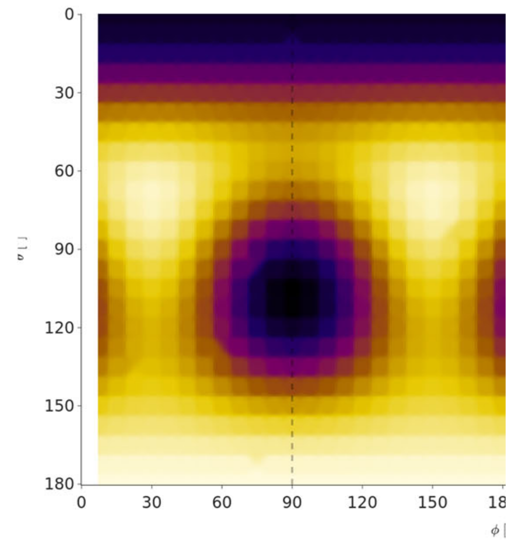
Wu et al. (2024). Deep-potential enabled multiscale simulation of gallium nitride devices on boron arsenide cooling substrates. *Nature Communications*, *15*(1), 2540.
Li et al. (2024). Deep learning interatomic potential for thermal and defect behaviour of aluminum nitride with quantum accuracy. *Computational Materials Science*, *232*, 112656.
Huang et al. (2023). First-principles based deep neural network force field for molecular dynamics simulation of N–Ga–Al semiconductors. *Physical Chemistry Chemical Physics*, *25*(3), 2349-2358.
Lei et al. (2023). Comparative studies of interatomic potentials for modeling point defects in wurtzite GaN. *AIP Advances*, *13*(1).
Zhu et al. (2023). Computational study of native defects and defect migration in wurtzite AlN: an atomistic approach. *Journal of Materials Chemistry A*, *11*(28), 15482-15498.

Next:
Theory of Radiation-induced Defects in Al-Ga-N

Threshold Displacement Energy (TDE) Study







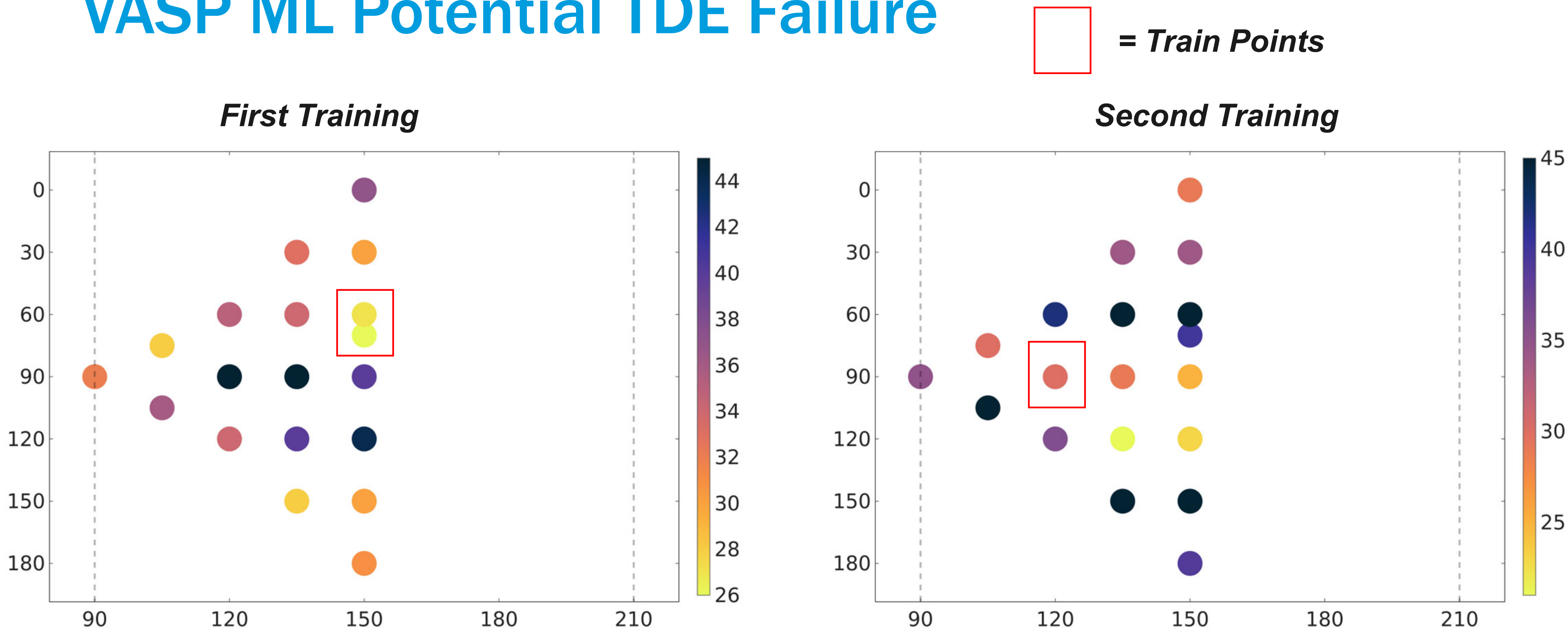
Appl. Phys. Lett. **124, 152107 (2024)**
https://doi.org/10.1063/5.0190371

Summary of Study

- Developed high-throughput computational TDE search tool
  - https://github.com/hauck-as/findTDE
- The calculated GaN TDE values agree with experiment
- N FP defects recombine → undetected by Luminescence
- Effect of lattice temperature reduces TDE by $\sim 1\ eV$
- New TDE values provided for AlN and Ga-rich AlGaN
- Al TDE in AlGaN sensitive to local environment but Ga not

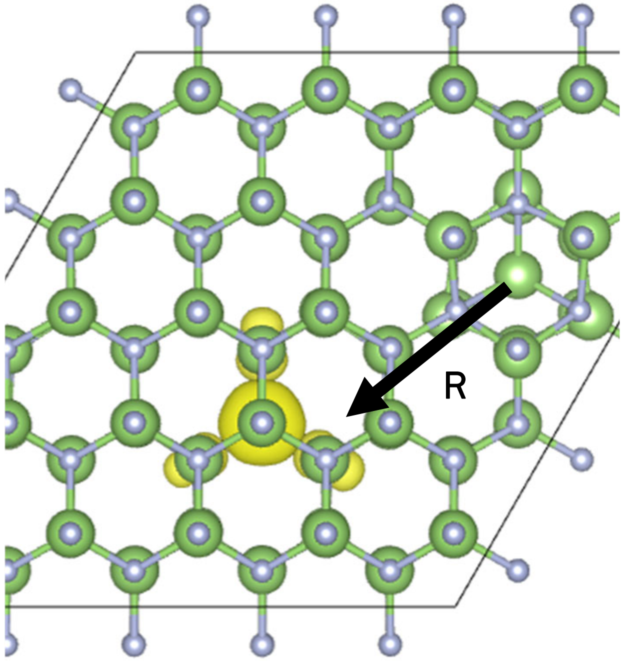
Appl. Phys. Lett. **124, 152107 (2024)**
https://doi.org/10.1063/5.0190371

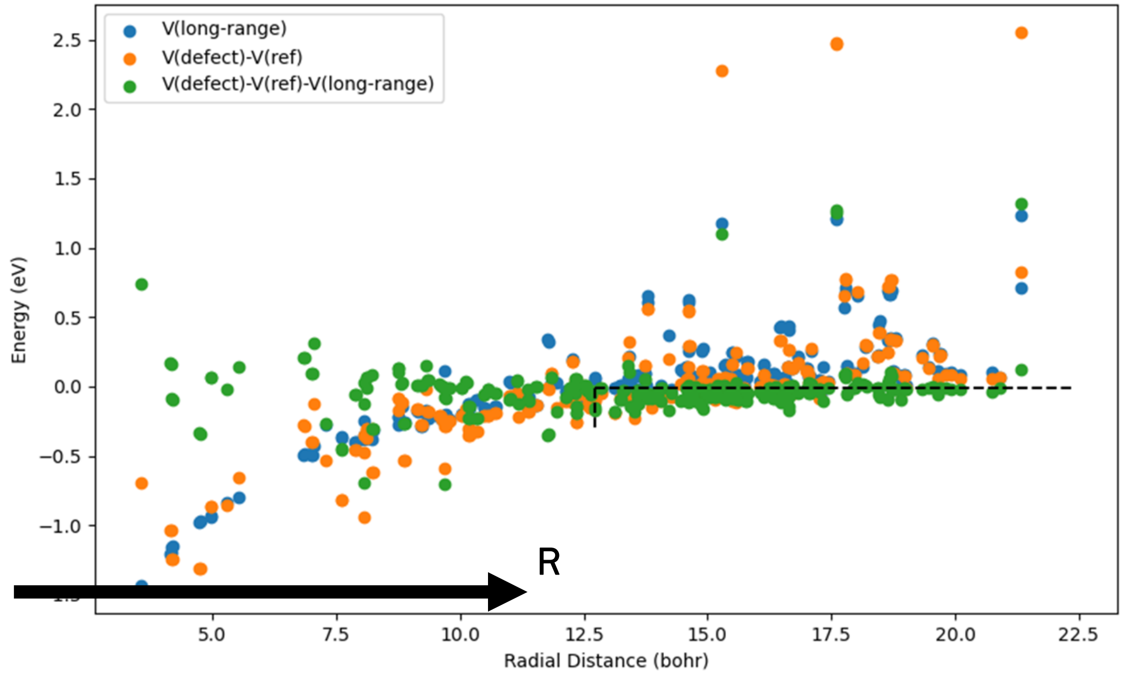
VASP ML Potential TDE Failure



Ga Frenkel Pair in GaN

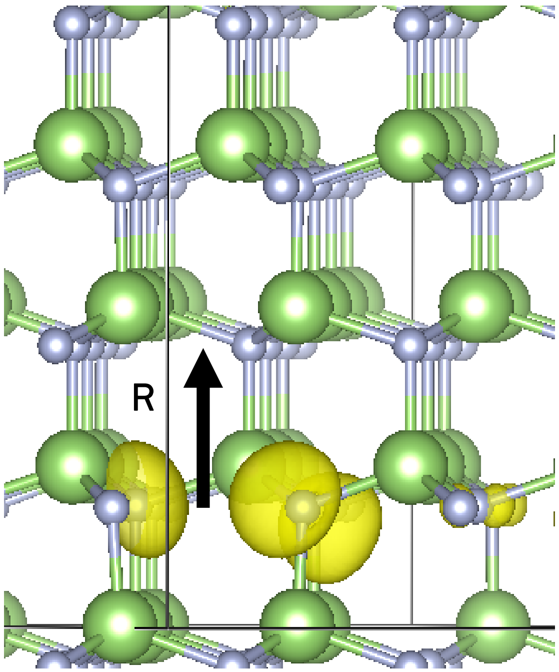
- Created model for electron transfer from Ga interstitial to Ga

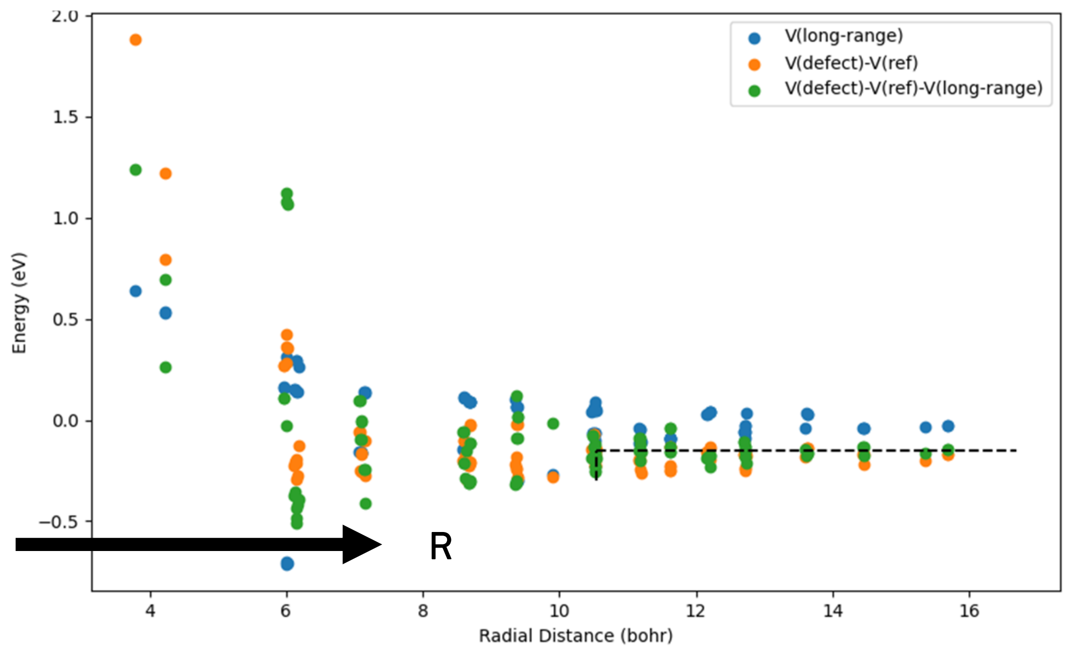




Vacancy Pair in GaN

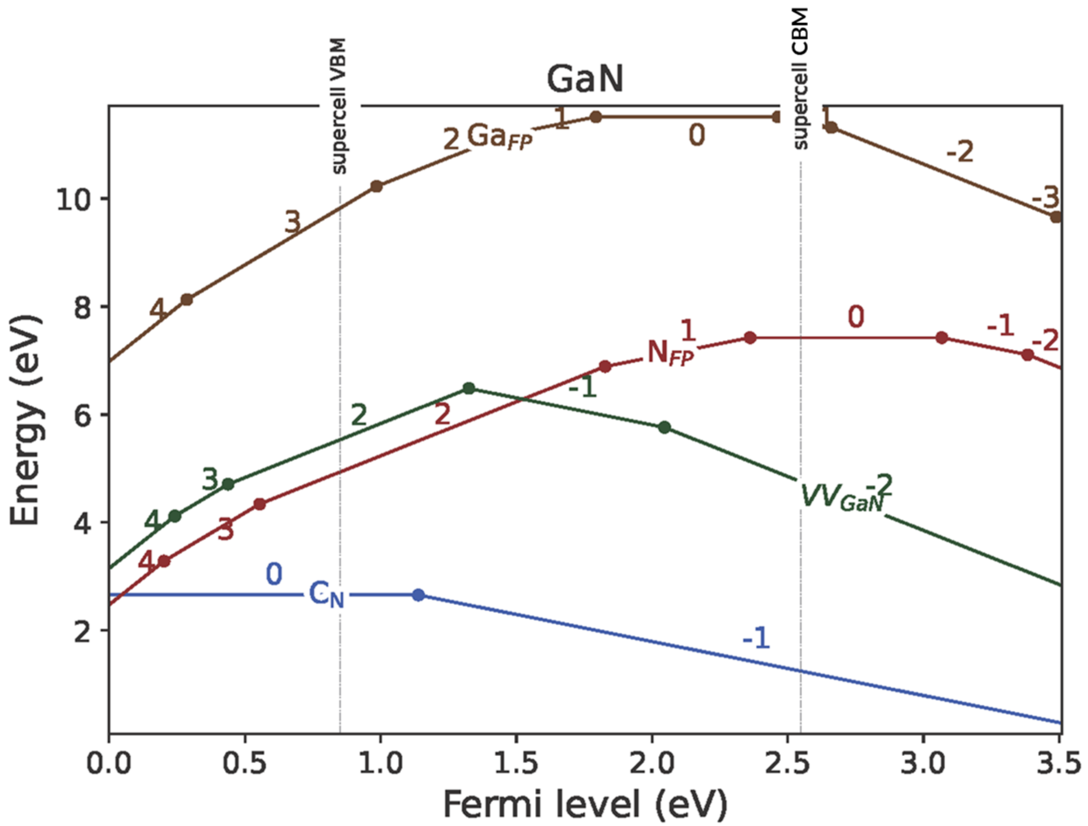
- Electrons transfer from N vacancy to Ga vacancy



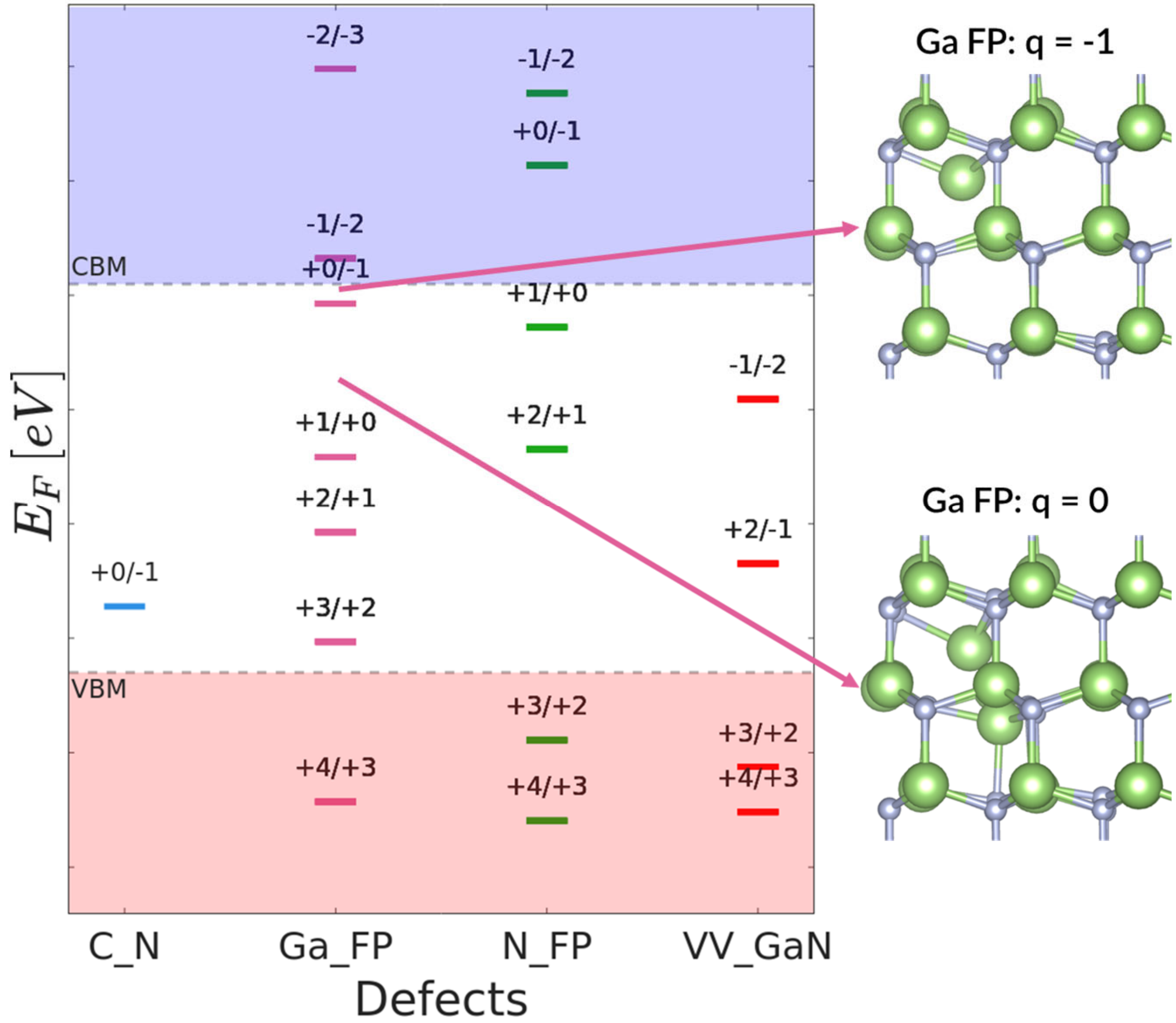


Defect formation energies

- First-principles formation energies show the most energetically favorable charge states (integer slopes) for each defect as a function of Fermi level across the band gap.

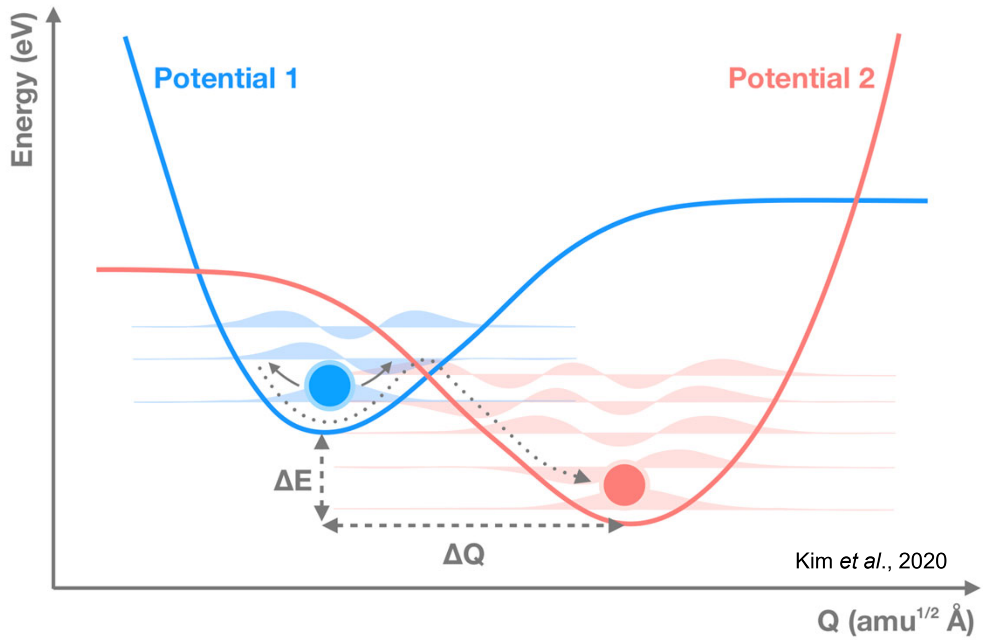


Charge transition levels



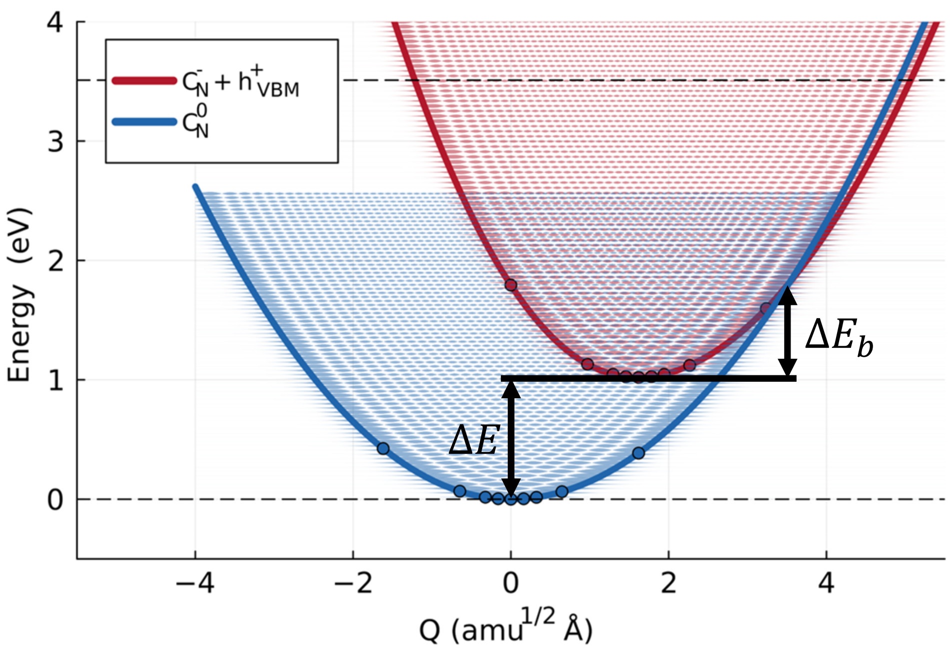
Carrier capture

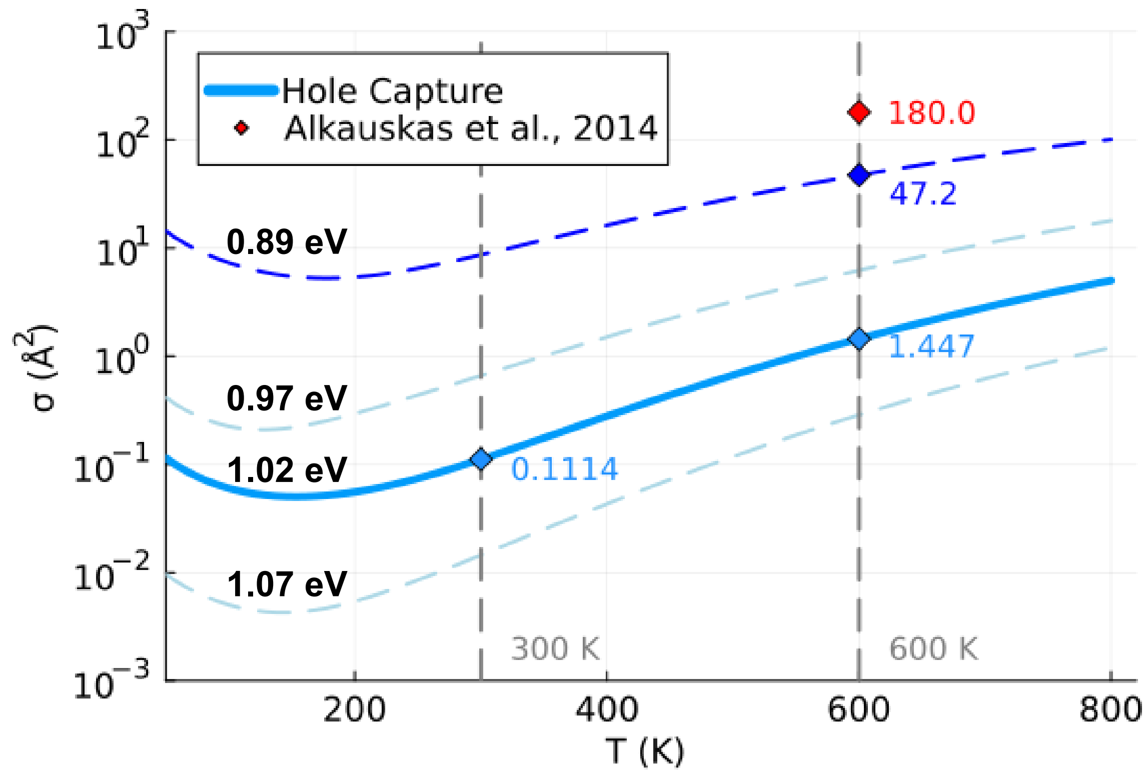
- Defects can introduce trap states into the electronic band gap which may enhance nonradiative recombination by several mechanisms utilizing metastable defect configurations.
- Franck-Condon Principle.
- Configuration coordinate diagrams show potential energy curves for interpolated/extrapolated structures between two equilibrium configurations, yielding energy barriers for transitions between the states.



C_N Capture Cross-Section

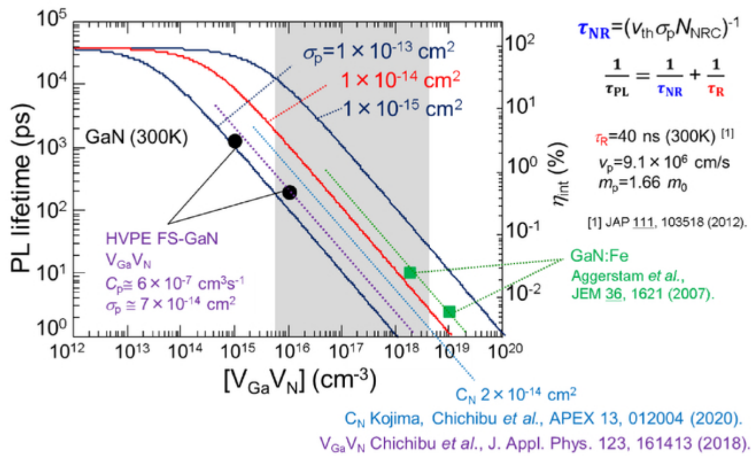
- Capture Cross-Section @ 600 K based on *Alkauskas et al.*, 2014: 180 Å^2
- Current result on capture cross-section @ 600 K: 47.2 Å^2





V_{Ga}–V_N Capture Cross-Sections

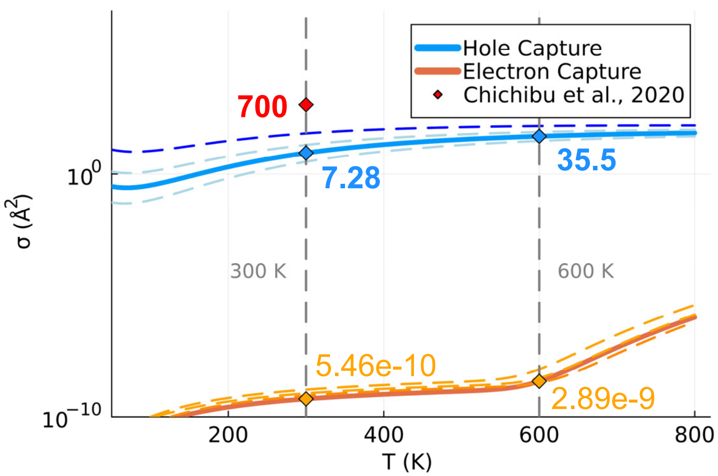
- Capture Cross-Section @ 300 K (Chichibu et al., 2020): 700 Å²



-1↔0

Hole Capture: 7.28 Å²

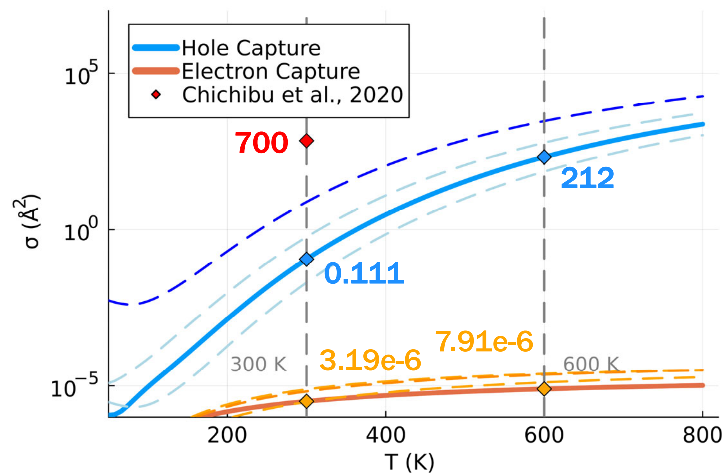
Electron Capture: 5.46e-10 Å²



-2↔-1

Hole Capture: 0.111 Å²

Electron Capture: 3.19e-6 Å²



Summary: theoretical and computational work

Poster by Farshid Reza:

Exploring Al/GaN Defects with Molecular Dynamics

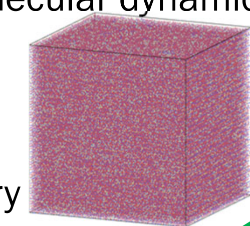
- Electronic effects
- Radiation-induced defects

- Electronic effects
- Defect properties
- Carrier capture cross-section

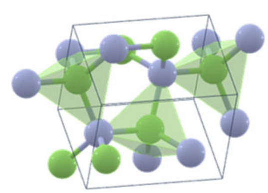
Poster by Alexander Hauck:

First-principles calculations of nonradiative carrier capture for defect complexes in AlGaN systems

- Molecular dynamics



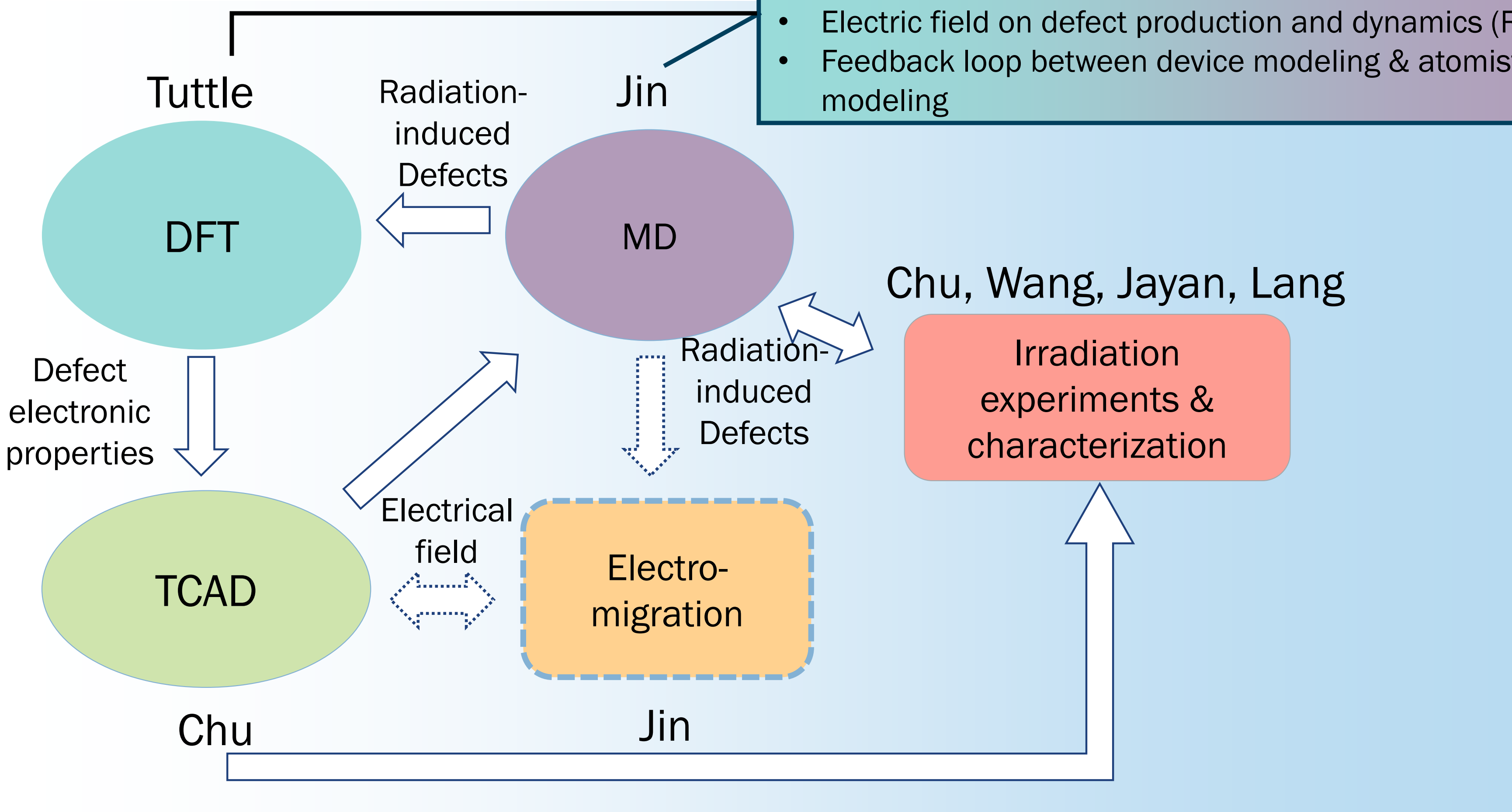
- Density functional theory

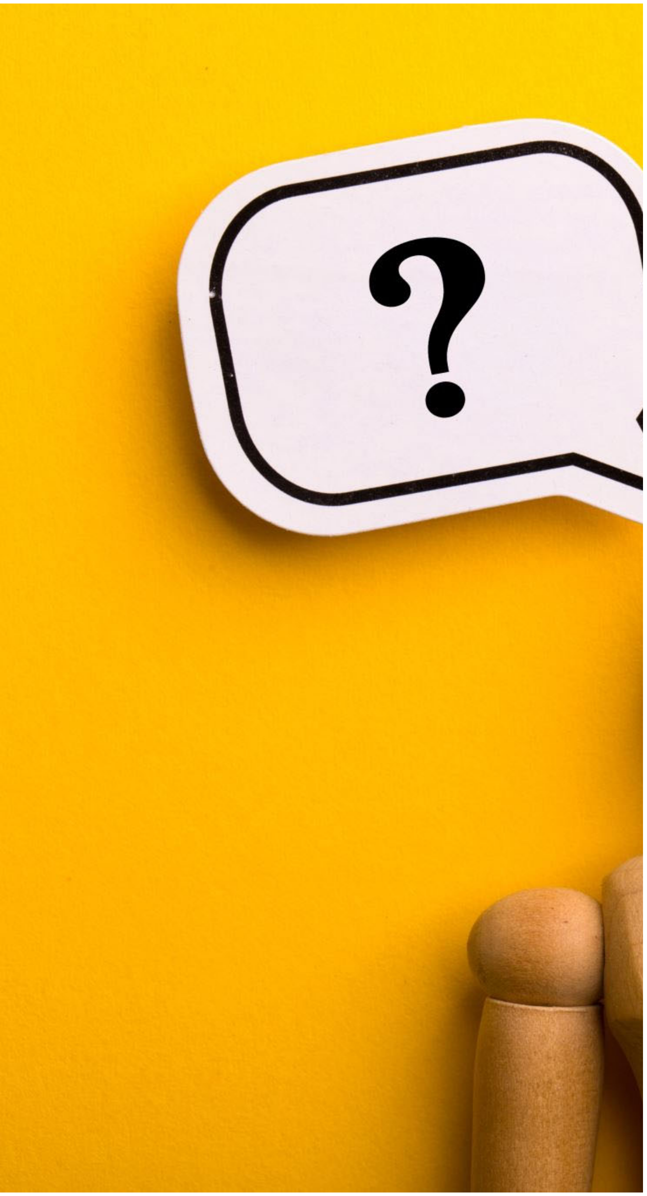


Time & Lenth

Relevant efforts & next steps

Upcoming key tasks:
- High-throughput evaluation of defect electronical properties
- Electric field on defect production and dynamics (ReaxFF)
- Feedback loop between device modeling & atomistic modeling





Thanks for your attention!

Mia Jin (mmjin@psu.edu)

2025 MRS® SPRING MEETING & EXHIBIT
April 7-11, 2025 | Seattle, Washington

CALL FOR PAPERS
Abstract Submission Opens Tuesday, September 17, 2024
Abstract Submission Closes Thursday, October 17, 2024 (11:59 PM ET)

Symposium EL04: Radiation Effects in Semiconductors for Extreme Environments -

Research on radiation effects in semiconductors for applications in extreme environments remains an active and crucial area of study. Radiation-hardening techniques are being actively explored to enhance the resilience of semiconductor devices against ionizing radiation, especially for applications in space, nuclear power plants, medical devices, and high-altitude aviation. Extensive efforts are concentrated on gaining a deeper understanding of the mechanisms by which ionizing radiation impacts semiconductor materials, encompassing studies on the effects of various radiation types, such as gamma rays, neutrons, and ions, on both the electronic and structural properties of semiconductors. In parallel, identifying or engineering semiconductor materials that inherently possess greater resistance to radiation-induced damage remains a focal point to address the need for radiation tolerance to ensure reliability. Device-level studies are also being conducted to assess the impact of radiation on the performance and reliability of specific semiconductor devices. The success of implementing radiation-hard semiconductor technologies relies on key breakthroughs and fundamental discoveries in semiconductor materials and device designs. This symposium hopes to bring together prominent efforts in this field. Particular emphasis will be laid on novel experimental and modeling approaches that approach radiation responses of (ultra)wide bandgap materials and devices.

Topics will include:

- Advanced experimental, modeling, and data-driven approaches to predict the effects of ionizing radiation
- Behavior and properties of radiation-induced defects
- Radiation-induced single-event effects
- Radiation-induced degradation of electronic performance
- Innovative strategies for enhancing the radiation hardness of semiconductor devices
- Novel semiconductor materials or modifications to existing materials to improve their inherent resistance to radiation-induced damage

Invited speakers include:

Ruben Alia Garcia	CERN, Switzerland	**Ani Khachatrian**	Naval Research Laboratory, USA
Aaron Arehart	Ohio State University, USA	**Andrew O'Hara**	Western Michigan University, USA
Scooter Ball	Vanderbilt University, USA	**Stephen Pearton**	University of Florida, USA
Stefano Bonaldo	University of Padova, Italy	**Miguel Sequeira**	Instituto Superior Técnico, Portugal
Rongming Chu	Pennsylvania State University, USA	**Blair Tuttle**	Pennsylvania State University, USA
Rosine Coq Germanicus	Université de Caen Normandie, France	**Chris Van de Walle**	University of California at Santa Barbara, USA
Esmat Farzana	Iowa State University, USA	**Grace Xing**	Cornell University, USA
Max Fischetti	University of Texas at Dallas, USA	**Enxia Zhang**	University of Central Florida, USA

Symposium Organizers

Miaomiao (Mia) Jin
Pennsylvania State University
Nuclear Engineering
USA
Tel (814) 865-4863, mmjin@psu.edu

Daniel M Fleetwood
Vanderbilt University
USA
Tel (615) 322-2498, dan.fleetwood@vanderbilt.edu

Ulrike Grossner
ETH Zürich
Switzerland
Tel (044)-632-2807, ulrike.grossner@ethz.ch

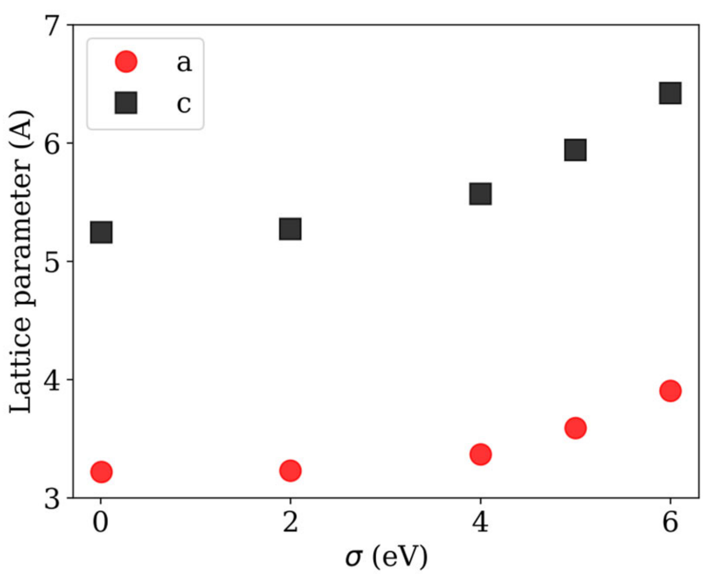
Tania Roy
Duke University
USA
Tel (919) 660-4215, tania.roy@duke.edu

Submission reopens: December 13, 2024 - January 8, 2025

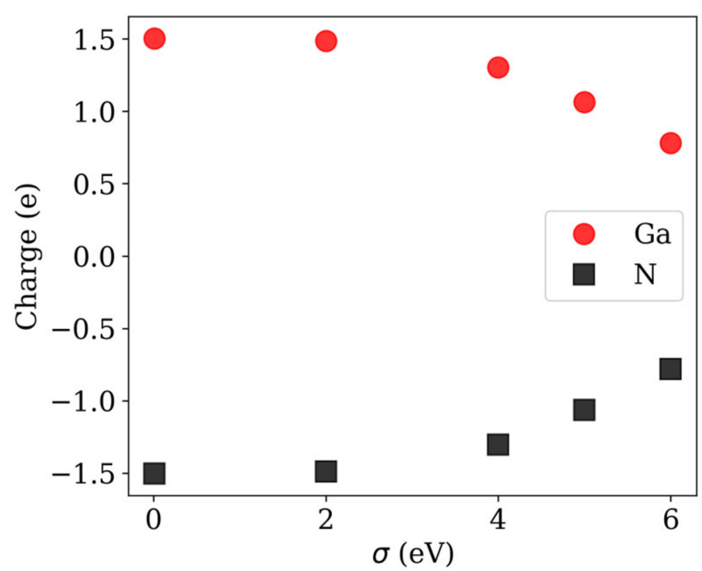
Effect of electron temperature

- GaN

Lattice parameter



Bader Charge analysis



Reduction of charges

Unit cell