

Supporting Information

A combined AIMD and DFT study of the low energy radiation responses of GaN

Ming Jiang^{1,*}, Nuo Cheng², Xin-Yu Zhu², Xuan-Liang Hu³, Zi-Han Wang³, Ning Liu³,
Shuo Song³, Sheng-Ze Wang³, Xu-Sheng Liu^{4,*}, Chandra Veer Singh^{5,6,*}

¹Institutes of Physical Science and Information Technology, Anhui University, Hefei
230601, China

²School of Materials Science and Engineering, Anhui University, Hefei, 230601,
China

³Stony Brook Institute at Anhui University, Anhui University, Hefei 230601, China

⁴College of Physics and Engineering Technology, Chengdu Normal University,
Chengdu 611130, China

⁵Department of Materials Science and Engineering, University of Toronto, 184
College Street, Suite 140, Toronto, ON M5S 3E4, Canada

⁶Department of Mechanical and Industrial Engineering, University of Toronto, 5
King's College Road, Toronto, ON M5S 3G8, Canada

Table S1. Lattice parameters of bulk Ga and N₂.

	Materials Projected ID	Space Group	a(Å)	b(Å)	c(Å)
GaN	mp-142	Cmce	4.41	7.84	4.54
N ₂	mp-154	<i>P</i> 2 ₁ 3	5.56	5.56	5.56

Table S2. Defect formation energy (eV) in GaN as a function of supercell size.

	$2 \times 2 \times 1$ (16)	$2 \times 2 \times 2$ (32)	$3 \times 3 \times 2$ (72)	$3 \times 3 \times 3$ (108)	$3 \times 3 \times 4$ (144)
V_{Ga}	6.50	6.47	6.34	6.34	6.33
V_{N}	3.03	3.02	2.95	2.90	2.92
Ga_{int}	8.74	8.58	8.47	8.51	8.42
N_{int}	4.07	4.01	3.91	3.87	3.85
Ga_{N}	5.91	5.91	5.80	5.79	5.77
N_{Ga}	6.98	6.84	6.71	6.67	6.62

Table S3 Lattice parameters of pristine and defective GaN.

	a (Å)	c (Å)	V
Pristine	9.69	10.50	853.82
V_N	9.68	10.50	852.07
V_{Ga}	9.65	10.49	845.98
N_{int}	9.78 (9.74)	10.54	866.44
Ga_{int}	9.72 (9.85)	10.60	878.68
N_{Ga}	9.68	10.49	851.25
Ga_N	9.74	10.62	871.75

Figure S1. Illustration of point defects at the end of Ga recoil events. The blue and grey spheres represent the Ga and N atoms, respectively. The red and yellow spheres represent the vacancy and interstitial defects.

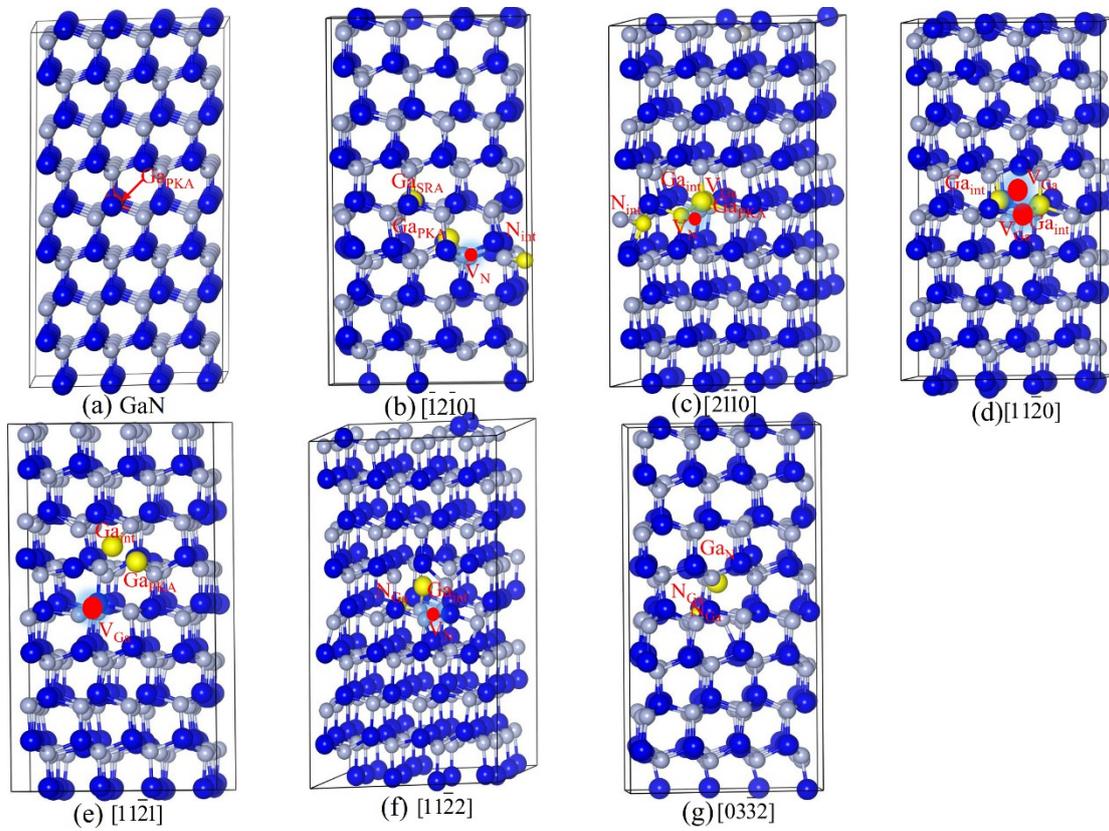


Figure S2. Illustration of point defects at the end of N recoil events. The blue and grey spheres represent the Ga and N atoms, respectively. The red and yellow spheres represent the vacancy and interstitial defects.

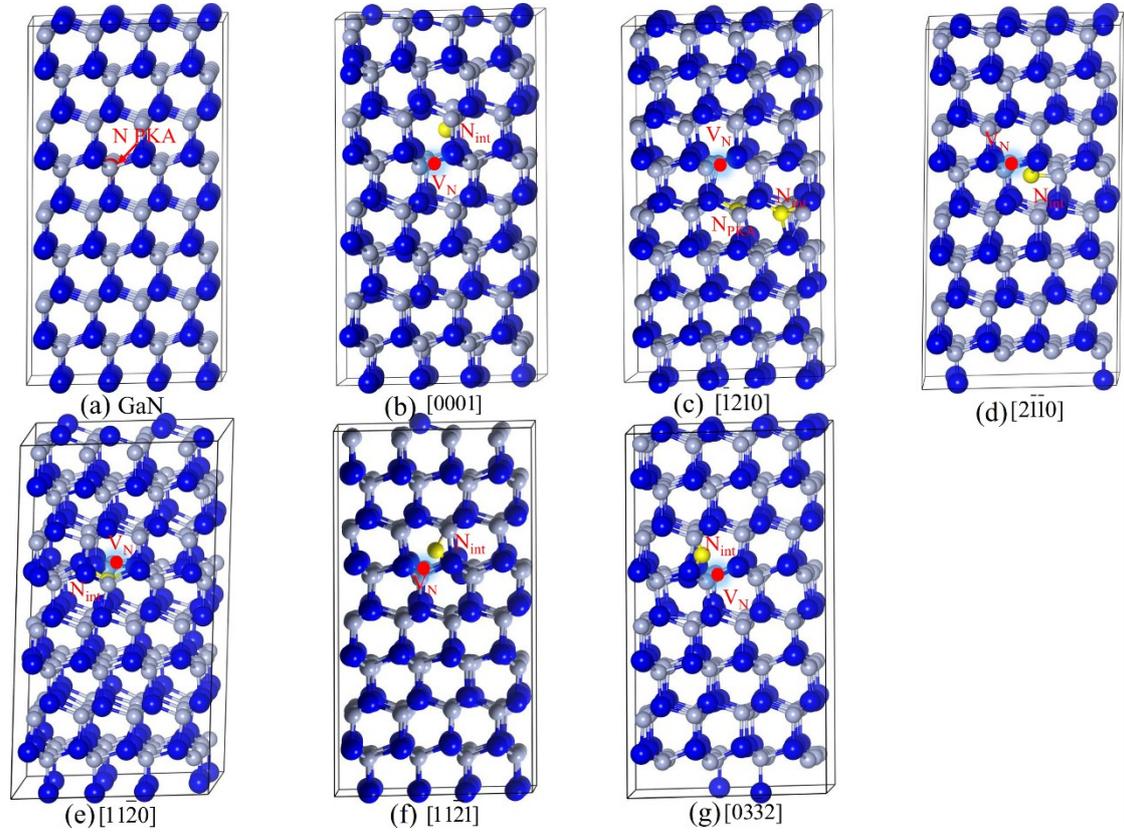


Figure S3. Variation of system temperature for GaN during the Ga recoil events.

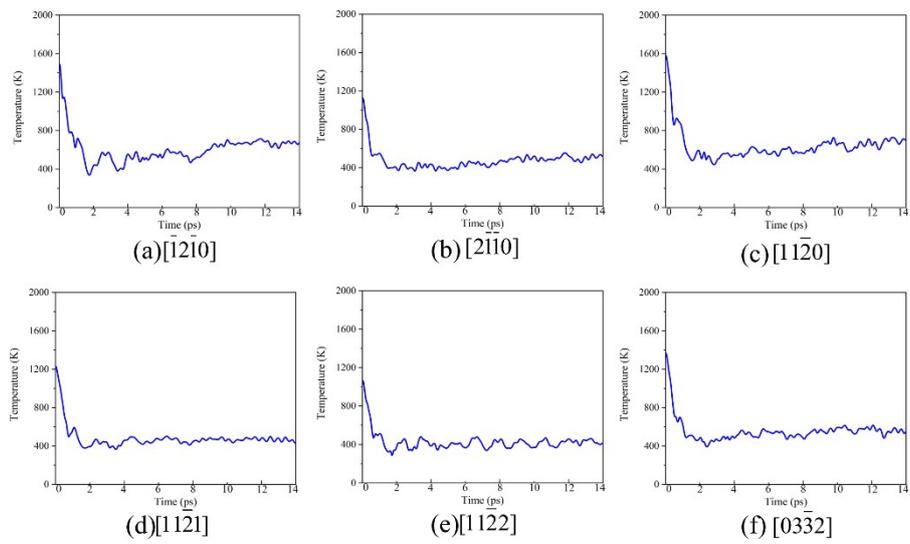


Figure S4. Variation of system temperature for GaN during the N recoil events.

