1 Primitive cell: Convergence tests

Table 1: Volumes of primitive cell for c-BN.

Structure	a (Å)	Volume
Perfect	2.56	11.958
Increase	2.58	12.240
Decrease	2.54	11.681

$$E^{rel}_{dec} = |E_{perf} - E_{dec}| \tag{1}$$

$$E^{rel}_{inc} = |E_{perf} - E_{inc}| \tag{2}$$

$$\Delta E^{rel}_{dec} = |E^{rel}_{dec}[i+1] - E^{rel}_{dec}[i]| \tag{3}$$

$$\Delta E^{rel}_{inc} = |E^{rel}_{inc}[i+1] - E^{rel}_{inc}[i]| \tag{4}$$

Table 2: Energy cutoff: Convergence test of primitive cell for c-BN. Criteria is 1 meV.

ENCUT (eV)	E_{perf} (eV)	E_{dec} (eV)	E_{inc} (eV)	E^{rel}_{dec} (meV)	E^{rel}_{inc} (meV)	ΔE^{rel}_{dec} (meV)	ΔE^{rel}_{inc} (meV)
200	-17.0024	-16.9378	-17.0416	64.6290	39.1838	–	–
250	-17.5246	-17.5200	-17.5383	4.6243	13.7043	60.0047	25.4795
300	-17.4699	-17.4620	-17.4607	7.8421	9.1176	3.2178	4.5867
350	-17.4260	-17.4170	-17.4157	8.9417	10.1970	1.0996	1.0794
400	-17.4490	-17.4468	-17.4407	2.1904	8.2843	6.7513	1.9127
450	-17.4542	-17.4483	-17.4452	5.9543	9.0336	3.7639	0.7493
500	-17.4513	-17.4455	-17.4420	5.7687	9.2785	0.1856	0.2449
550	-17.4517	-17.4461	-17.4424	5.6772	9.3078	0.0915	0.0293
600	-17.4545	-17.4488	-17.4450	5.6520	9.4998	0.0252	0.1920
650	-17.4567	-17.4512	-17.4472	5.5594	9.5653	0.0926	0.0655
700	-17.4582	-17.4527	-17.4487	5.5391	9.5108	0.0203	0.0545
750	-17.4591	-17.4535	-17.4496	5.5855	9.4552	0.0464	0.0556
800	-17.4597	-17.4540	-17.4503	5.6308	9.4063	0.0453	0.0489
850	-17.4599	-17.4543	-17.4505	5.6572	9.4013	0.0264	0.0050
900	-17.4600	-17.4543	-17.4506	5.6599	9.4011	0.0028	0.0001
950	-17.4601	-17.4544	-17.4507	5.6605	9.3973	0.0006	0.0038

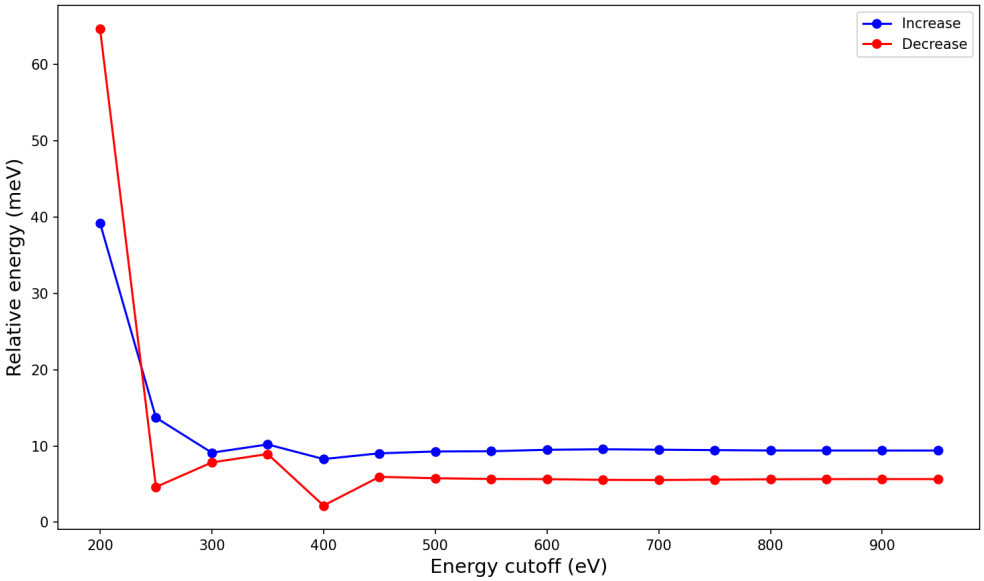

Figure 1: Convergence test of primitive cell for c-BN.

Table 3: K-density: Convergence test of primitive cell for c-BN. Criteria is 1 meV.

K-density (1/Å^3)	E_{perf} (eV)	E_{dec} (eV)	E_{inc} (eV)	E^{rel}_{dec} (meV)	E^{rel}_{inc} (meV)	ΔE^{rel}_{dec} (meV)	ΔE^{rel}_{inc} (meV)
2	-17.4348	-17.4288	-17.4259	6.0799	8.9643	–	–
3	-17.4510	-17.4452	-17.4418	5.8184	9.2433	0.2615	0.2790
4	-17.4513	-17.4455	-17.4420	5.7687	9.2785	0.0497	0.0352
5	-17.4513	-17.4455	-17.4420	5.7838	9.2641	0.0151	0.0144
6	-17.4513	-17.4455	-17.4420	5.7887	9.2551	0.0049	0.0090
7	-17.4513	-17.4455	-17.4420	5.7923	9.2623	0.0036	0.0072
8	-17.4513	-17.4455	-17.4420	5.7890	9.2603	0.0033	0.0020
9	-17.4513	-17.4455	-17.4420	5.7880	9.2638	0.0010	0.0034

Table 4: Kpoints mesh of primitive cell for c-BN

K-density (1/Å^3)	Kpoints mesh
2	$5 \times 5 \times 5$
3	$8 \times 8 \times 8$
4	$10 \times 10 \times 10$
5	$13 \times 13 \times 13$
6	$15 \times 15 \times 15$
7	$18 \times 18 \times 18$
8	$20 \times 20 \times 20$
9	$23 \times 23 \times 23$

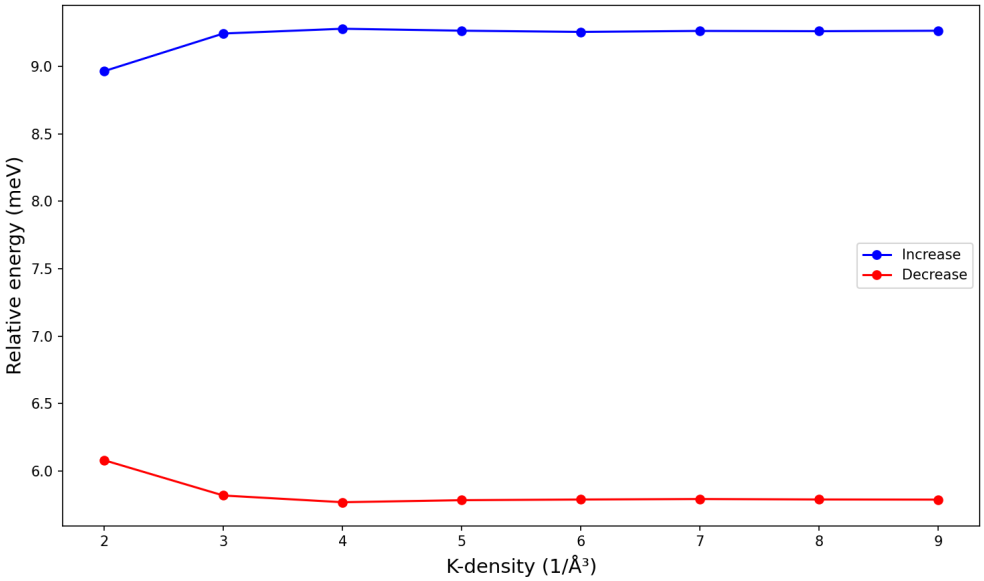

Figure 2: Convergence test of primitive cell for c-BN.

2 Convergence test: Stable phases

It also was calculated using the volumes, modifiying the lattice parameters: $\Delta a = \pm 0.02$.

2.1 Boron

Table 5: Energy cutoff: Convergence test of boron. Criteria is 1 meV.

ENCUT (eV)	E_{perf} (eV)	E_{dec} (eV)	E_{inc} (eV)	E_{dec}^{rel} (meV)	E_{inc}^{rel} (meV)	ΔE_{dec}^{rel} (meV)	ΔE_{inc}^{rel} (meV)
200	-78.6696	-78.6207	-78.6963	48.8942	26.7108	–	–
250	-79.8598	-79.8543	-79.8489	5.4990	10.8634	43.3952	15.8474
300	-80.2543	-80.2398	-80.2543	14.4919	0.0024	8.9929	10.8610
350	-80.4190	-80.4018	-80.4173	17.1116	1.6907	2.6197	1.6883
400	-80.4372	-80.4209	-80.4352	16.3599	1.9767	0.7517	0.2860
450	-80.4363	-80.4199	-80.4342	16.3471	2.0519	0.0128	0.0752
500	-80.4404	-80.4243	-80.4381	16.0692	2.3424	0.2779	0.2905
550	-80.4460	-80.4301	-80.4436	15.9086	2.4194	0.1606	0.0770
600	-80.4531	-80.4372	-80.4507	15.9103	2.3978	0.0017	0.0216
650	-80.4593	-80.4434	-80.4569	15.9044	2.4684	0.0059	0.0707
700	-80.4631	-80.4472	-80.4606	15.8750	2.4987	0.0294	0.0302
750	-80.4647	-80.4488	-80.4621	15.8515	2.5468	0.0234	0.0481
800	-80.4651	-80.4493	-80.4625	15.8085	2.5706	0.0431	0.0238
850	-80.4652	-80.4494	-80.4626	15.7976	2.5815	0.0109	0.0109
900	-80.4654	-80.4496	-80.4628	15.7855	2.5935	0.0121	0.0120
950	-80.4659	-80.4501	-80.4633	15.7921	2.5953	0.0067	0.0018

Table 6: K-density: Convergence test of boron. Criteria is 1 meV.

K-density (1/Å^3)	E_{perf} (eV)	E_{dec} (eV)	E_{inc} (eV)	E_{dec}^{rel} (meV)	E_{inc}^{rel} (meV)	ΔE_{dec}^{rel} (meV)	ΔE_{inc}^{rel} (meV)
2	-80.4923	-80.4760	-80.4898	16.2435	2.4457	–	–
3	-80.4276	-80.4113	-80.4255	16.3307	2.0707	0.0873	0.3750
4	-80.4342	-80.4199	-80.4354	16.3471	2.0519	0.0163	0.0188
5	-80.4375	-80.4212	-80.4355	16.3470	2.0716	0.0001	0.0198
6	-80.4375	-80.4212	-80.4355	16.3368	2.0831	0.0102	0.0114
7	-80.4375	-80.4212	-80.4355	16.3522	2.0772	0.0154	0.0059
8	-80.4375	-80.4212	-80.4355	16.3443	2.0709	0.0079	0.0064
9	-80.4375	-80.4212	-80.4355	16.3380	2.0667	0.0063	0.0042

Table 7: Kpoints mesh for boron (mp-160).

K-density (1/Å^3)	Kpoints mesh
2	$3 \times 3 \times 3$
3	$4 \times 4 \times 4$
4	$5 \times 5 \times 5$
5	$7 \times 7 \times 7$
6	$8 \times 8 \times 8$
7	$9 \times 9 \times 9$
8	$10 \times 10 \times 10$
9	$12 \times 12 \times 12$

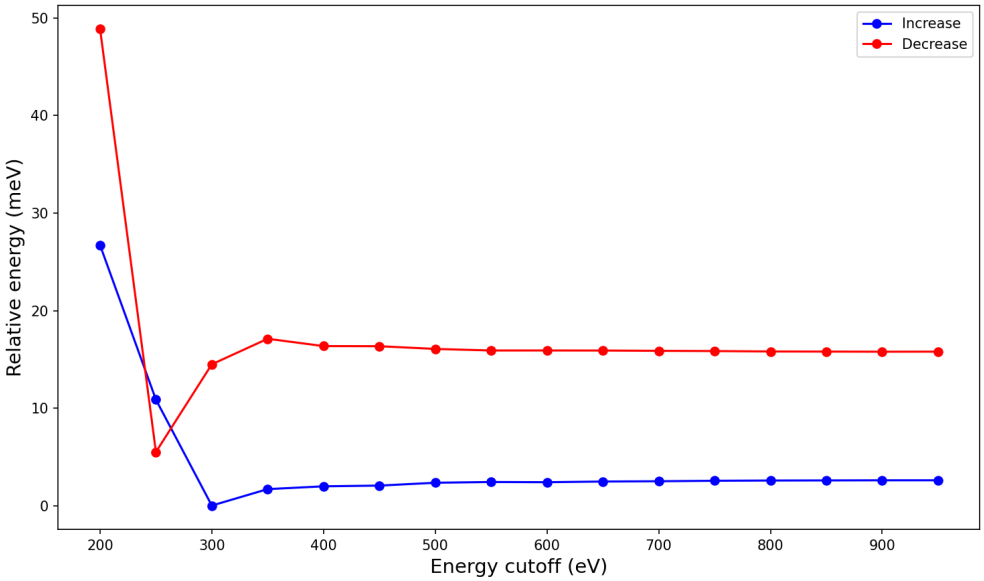

Figure 3: Convergence test of boron.

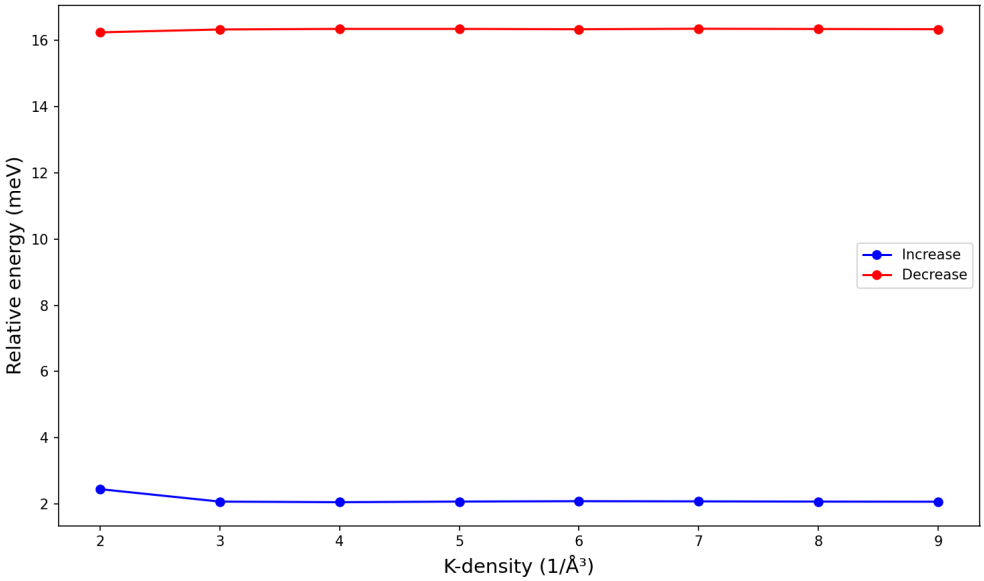

Figure 4: Convergence test of boron.

2.2 Nitrogen

Table 8: Energy cutoff: Convergence test of nitrogen. Criteria is 1 meV.

ENCUT (eV)	E_{perf} (eV)	E_{dec} (eV)	E_{inc} (eV)	E^{rel}_{dec} (meV)	E^{rel}_{inc} (meV)	ΔE^{rel}_{dec} (meV)	ΔE^{rel}_{inc} (meV)
200	-17.2558	-17.2318	-17.2195	24.0068	36.2361	–	–
250	-16.6474	-16.6301	-16.6489	17.3020	1.4754	6.7049	34.7608
300	-16.4950	-16.4872	-16.4993	7.7920	4.3531	9.5100	2.8778
350	-16.5192	-16.5103	-16.5228	8.8587	3.5650	1.0667	0.7882
400	-16.5906	-16.5837	-16.5946	6.8461	3.9972	2.0126	0.4322
450	-16.6146	-16.6101	-16.6188	4.4686	4.2182	2.3775	0.2210
500	-16.6232	-16.6188	-16.6267	4.3515	3.5494	0.1171	0.6688
550	-16.6285	-16.6243	-16.6318	4.1817	3.3163	0.1699	0.2331
600	-16.6332	-16.6291	-16.6363	4.0529	3.1872	0.1288	0.1292
650	-16.6366	-16.6326	-16.6398	3.9907	3.1911	0.0622	0.0040
700	-16.6389	-16.6350	-16.6421	3.9576	3.1518	0.0331	0.0394
750	-16.6399	-16.6359	-16.6430	3.9074	3.1653	0.0502	0.0135
800	-16.6406	-16.6367	-16.6437	3.9270	3.1215	0.0196	0.0438
850	-16.6410	-16.6371	-16.6441	3.9195	3.1240	0.0076	0.0025
900	-16.6413	-16.6374	-16.6444	3.8977	3.1113	0.0217	0.0127
950	-16.6417	-16.6378	-16.6448	3.8852	3.1017	0.0126	0.0095

Table 9: K-density: Convergence test of nitrogen. Criteria is 1 meV. We can note that gases are independent of the kdensity or kpoints mesh. The Γ-point only calculation is sufficient.

K-density (1/Å^3)	E_{perf} (eV)	E_{dec} (eV)	E_{inc} (eV)	E^{rel}_{dec} (meV)	E^{rel}_{inc} (meV)	ΔE^{rel}_{dec} (meV)	ΔE^{rel}_{inc} (meV)
1	-16.6233	-16.6193	-16.6267	4.0180	3.3979	–	–
2	-16.6233	-16.6188	-16.6268	4.4684	3.5690	0.4504	0.1711
4	-16.6232	-16.6188	-16.6267	4.3515	3.5494	0.1169	0.0196
5	-16.6231	-16.6188	-16.6267	4.3198	3.5666	0.0318	0.0172
7	-16.6232	-16.6188	-16.6267	4.3258	3.5164	0.0061	0.0502
8	-16.6232	-16.6188	-16.6267	4.3391	3.5305	0.0133	0.0141

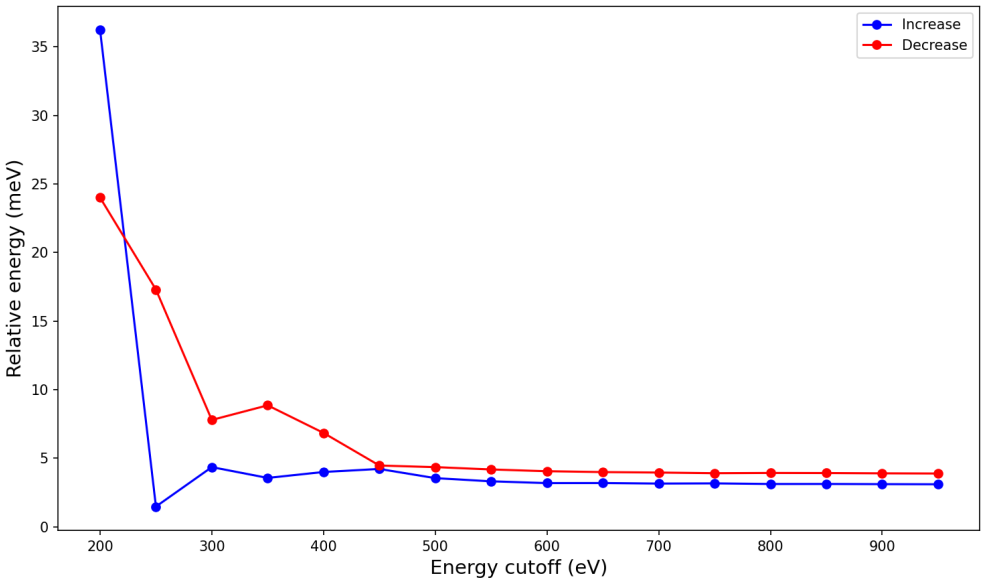

Figure 5: Convergence test of nitrogen.

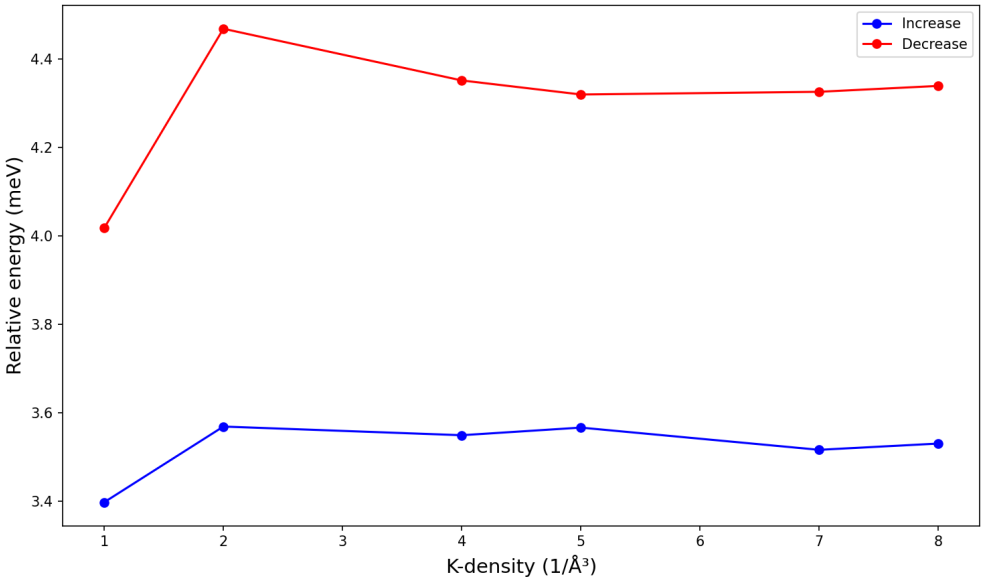

Figure 6: Convergence test of nitrogen.

3 Chemical potentials: Stable phases

Table 10: Boron and nitrogen structures.

Species	Total energy (eV)	Number of atoms	$\mu_i^{elemental}$ (eV)
Boron	-80.43	12	-6.70
Nitrogen	-16.63	2	-8.31

4 Convergence for supercell size

$$E_{form}^{q=0} = E_{def}^{q=0} - E_{perf} + \mu_i^{elemental} \tag{5}$$

Table 11: Convergence test of supercell size for c-BN.

N	E_{perf} (eV)	$E_{def}[V_B]$ (eV)	$E_{def}[V_N]$ (eV)	$E_{form}[V_B]$ (eV)	$E_{form}[V_N]$ (eV)
64	-558.450	-542.435	-542.054	9.311	8.071
216	-1884.780	-1868.495	-1868.242	9.581	8.212
512	-4467.653	-4451.32	-4451.095	9.628	8.232
1000	-8725.994	-8709.647	-8709.423	9.643	8.245
1728	-15078.619	-15062.268	-15062.042	9.647	8.251

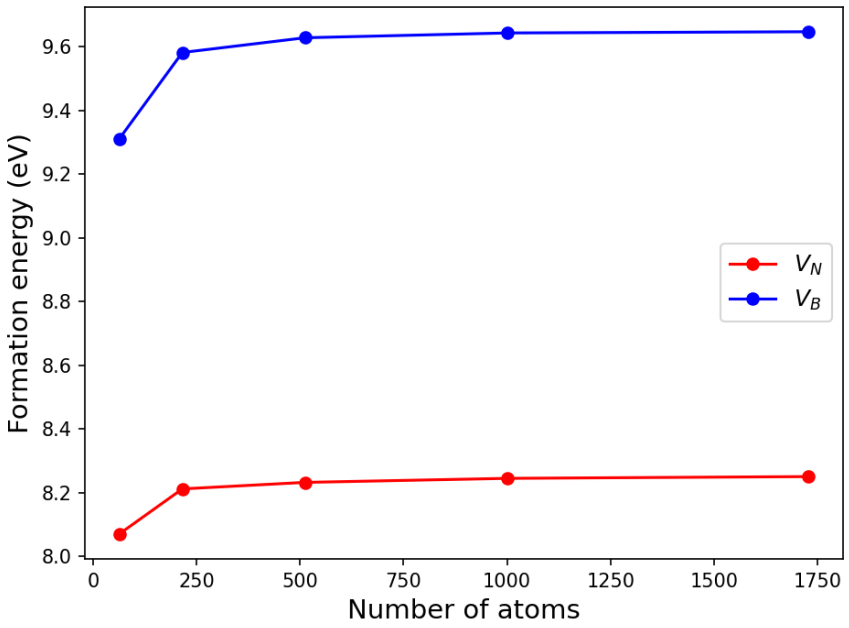

Figure 7: Convergence test on supercell size for native vacancies.

5 Supercell: Convergence tests

Using supercell with 216 atoms for nitrogen vacancy (V_N^0). Keep in mind the **Eq. 5**.

Table 12: Energy cutoff: Convergence test of supercell for nitrogen vacancy (V_N^0)

ENCUT (eV)	E_{perf} (eV)	$E_{def}[V_N^0]$ (eV)	E_{form} (eV)	ΔE_{form} (meV)
200	-1834.115	-1818.842	6.963	–
250	-1893.042	-1876.577	8.155	1.192
300	-1886.670	-1870.314	8.046	0.109
350	-1881.787	-1865.501	7.976	0.070
400	-1884.291	-1867.965	8.016	0.040
450	-1884.546	-1868.208	8.028	0.012
500	-1884.225	-1867.889	8.026	0.002
550	-1884.296	-1867.959	8.026	0.001
600	-1884.593	-1868.255	8.029	0.002
650	-1884.875	-1868.535	8.030	0.002
700	-1885.008	-1868.667	8.031	0.001
750	-1885.077	-1868.736	8.031	0.000
800	-1885.177	-1868.834	8.032	0.001
850	-1885.182	-1868.840	8.032	0.000
900	-1885.194	-1868.852	8.032	0.000
950	-1885.243	-1868.901	8.033	0.000

Table 13: K-density: Convergence test of supercell for nitrogen vacancy (V_N^0).

K-density (1/Å^3)	E_{perf} (eV)	$E_{def}[V_N^0]$ (eV)	E_{form} (eV)	ΔE_{form} (meV)
1	-1884.225	-1867.889	8.026	–
2	-1884.766	-1868.411	8.045	0.019
4	-1884.765	-1868.409	8.046	0.001
6	-1884.765	-1868.409	8.046	0.000
7	-1884.764	-1868.409	8.046	0.000
9	-1884.765	-1868.409	8.046	0.000

Table 14: Kpoints mesh for supercell.

K-density ($1/Å^3$)	Kpoints mesh
1	$1 \times 1 \times 1$
2	$2 \times 2 \times 2$
3	$2 \times 2 \times 2$
4	$3 \times 3 \times 3$
5	$3 \times 3 \times 3$
6	$4 \times 4 \times 4$
7	$5 \times 5 \times 5$
8	$5 \times 5 \times 5$
9	$6 \times 6 \times 6$

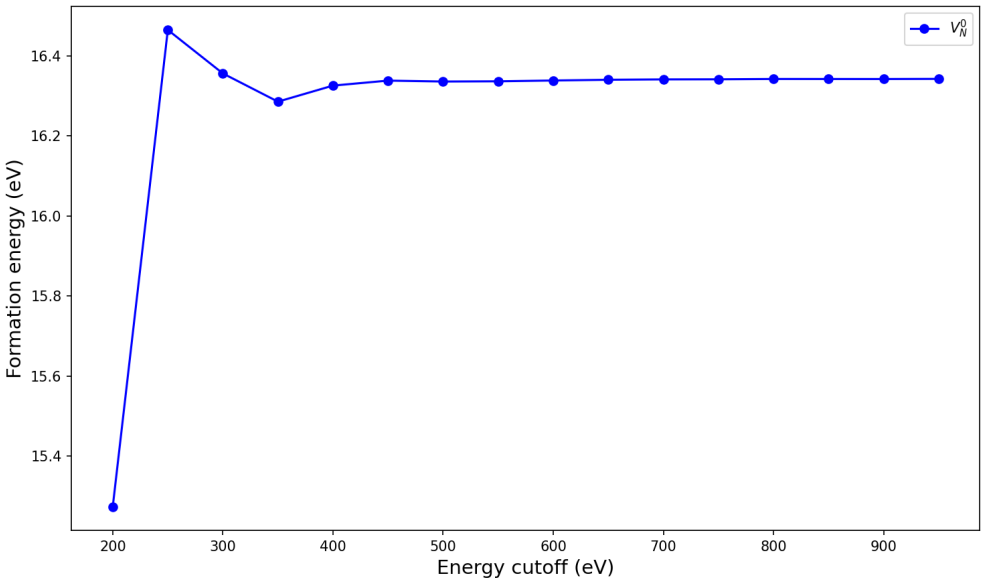

Figure 8: Convergence test of supercell for nitrogen vacancy (V_N^0).

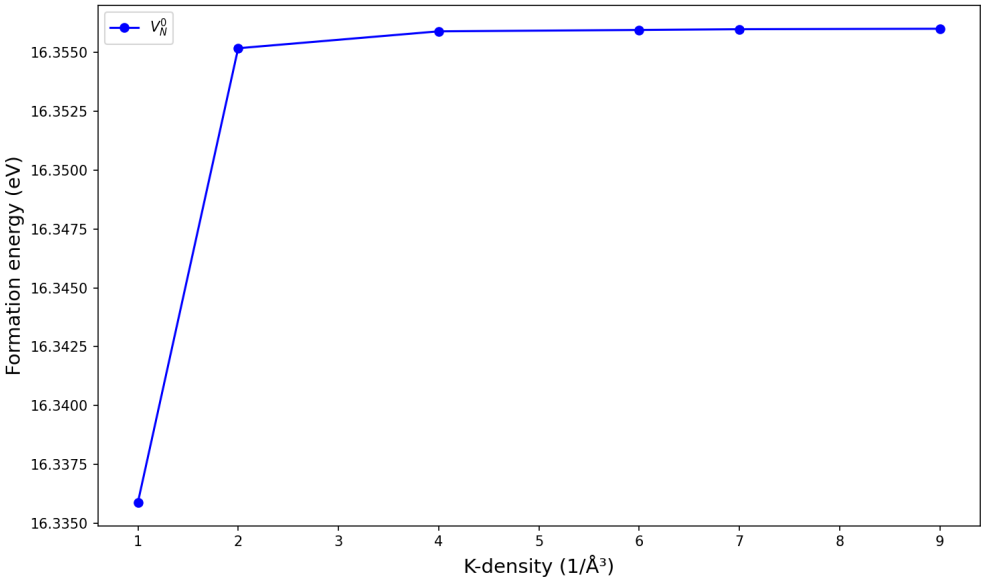

Figure 9: Convergence test of supercell for nitrogen vacancy (V_N^0).