Supporting Information: Atomistic simulation of HF etching process of amorphous Si_3N_4 using machine learning potential

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Table S1: Cutoff distances for each element pair used in the switching function.

Pair of elements	r_c^{in} (Å)	r_c^{out} (Å)
Si-Si	1.94	2.05
Si-N	1.34	1.42
Si-H	1.31	1.39
Si-F	1.39	1.47
N-N	0.95	1.0
N-H	0.89	0.95
N-F	1.14	1.21
H-H	0.64	0.68
H-F	0.8	0.84
F-F	1.21	1.28

Table S2: Parameters used in the symmetry functions for each element.

SF type	e_c	e_1	e_2	r_c (Å)	η (Å^{-2})	λ	ζ	# of SFs
G^2	Si, N	Si, N	-	6.0	0.003214, 0.035711, 0.071421, 0.124987, 0.214264, 0.357106, 0.714213, 1.42842	-	-	16
G^2	Si, N	H, F	-	4.5	0.003214, 0.071421, 0.214264, 0.714213	-	-	8
G^2	H, F	Si, N, H, F	-	4.5	0.003214, 0.071421, 0.214264, 0.714213	-	-	16
G^4	Si, N	Si, N	Si, N	4.5	0.000357, 0.028569, 0.089277	1, 2, 4	-1, 1	54
G^4	Si, N	Si, N	H, F	4.5	0.000357	1, 2, 4	-1, 1	24
G^4	Si, N	H, F	H, F	4.5	0.000357	1, 2, 4	-1, 1	18
G^4	H, F	Si, N, H, F	Si, N, H, F	4.5	0.000357	1, 2, 4	-1, 1	60

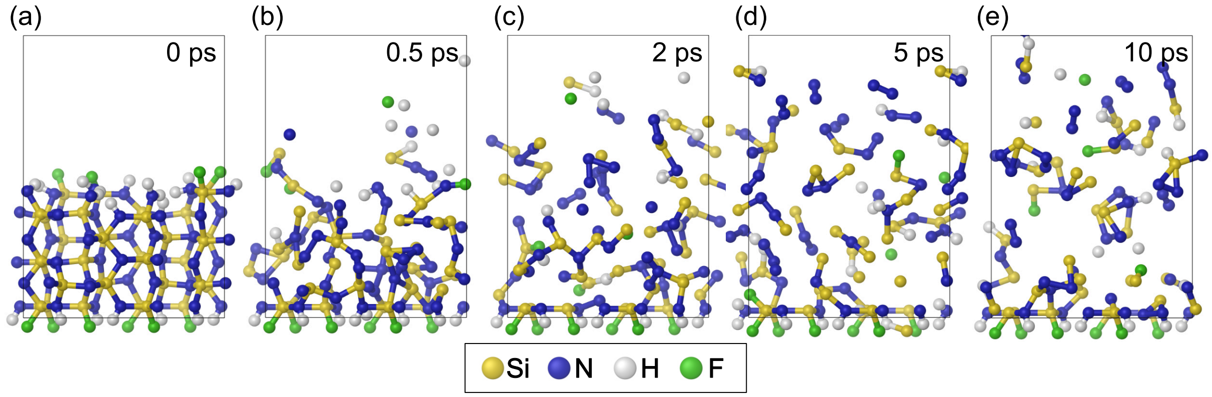

Figure S1: (a–e) Snapshots of high-temperature molecular dynamics (10 000 K) of the slab at $t = 0$, 0.5, 2, 5, 10 ps.

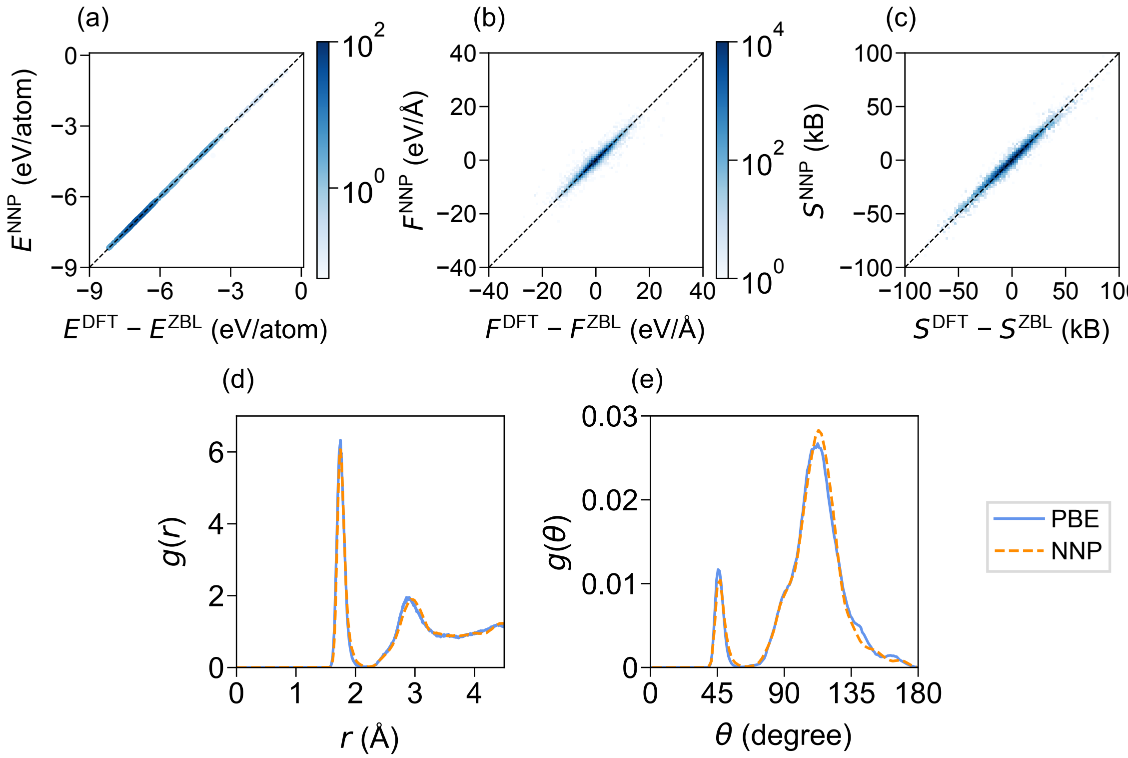

Figure S2: (a–c) Parity plots of energy, force component, and stress component of the test set. (d) Radial distribution function (RDF) and (e) angular distribution function (ADF) of amorphous Si_3N_4 obtained from the NNP and DFT calculations.

Table S3: Etching yields of H-terminated and pristine amorphous Si_3N_4 (a-Si_3N_4) substrates under various ion incidence conditions.

Incident energy (eV)	**Incident angle (°)**	**Substrate**	**Yield (Si_3N_4/HF)**
20	0	H-terminated	0.040
		Pristine	0.039
50	0	H-terminated	0.067
		Pristine	0.071
50	75	H-terminated	0.026
		Pristine	0.028

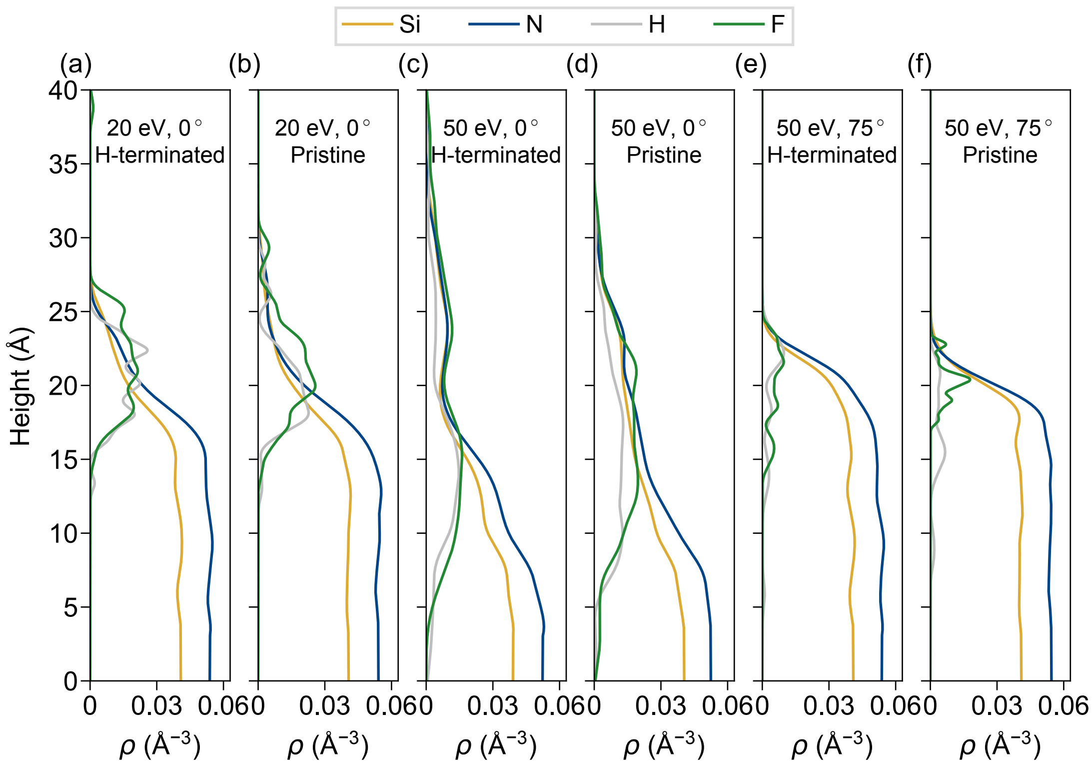

Figure S3: Surface profiles of H-terminated and pristine a-Si_3N_4 substrates after etching simulations under (a, b) E_{in} = 20 eV, θ_{in} = 0°; (c, d) E_{in} = 50 eV, θ_{in} = 0°; (e, f) E_{in} = 50 eV, θ_{in} = 75°. Panels (a, c, e) show H-terminated cases, while panels (b, d, f) show pristine cases.

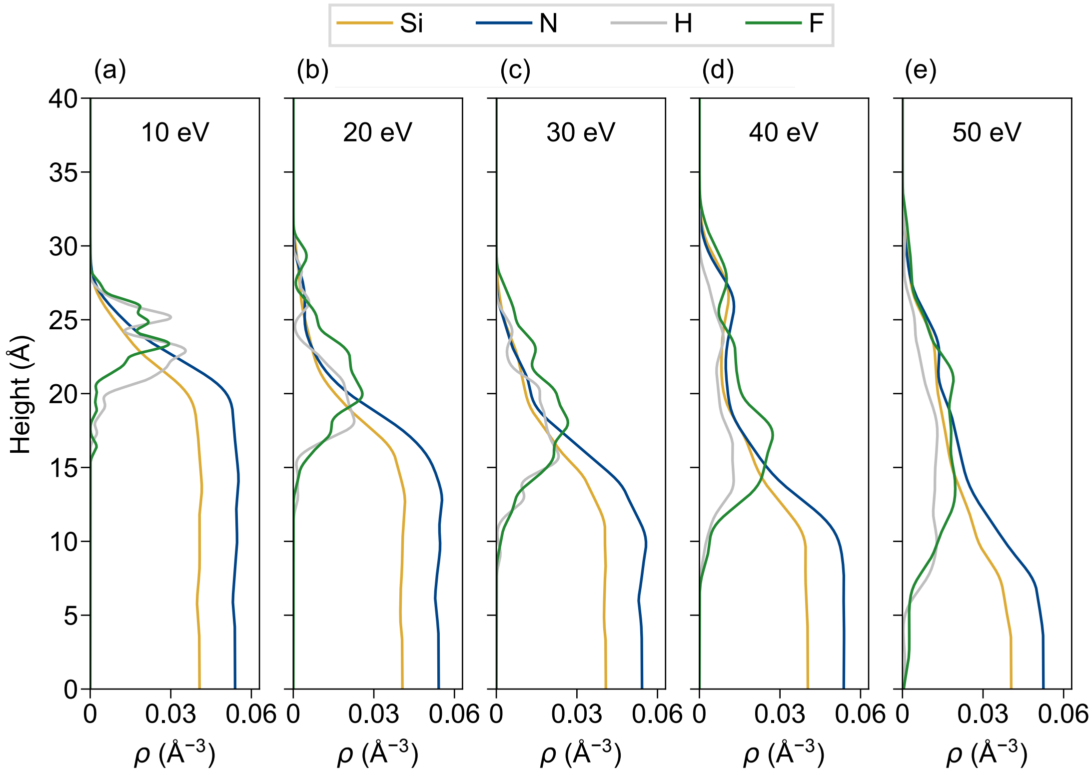

Figure S4: (a–e) Atomic density profiles of Si, N, H, and F for surfaces after the etching simulation under $E_{\mathrm{in}} = 10, 20, 30, 40, 50$ eV.

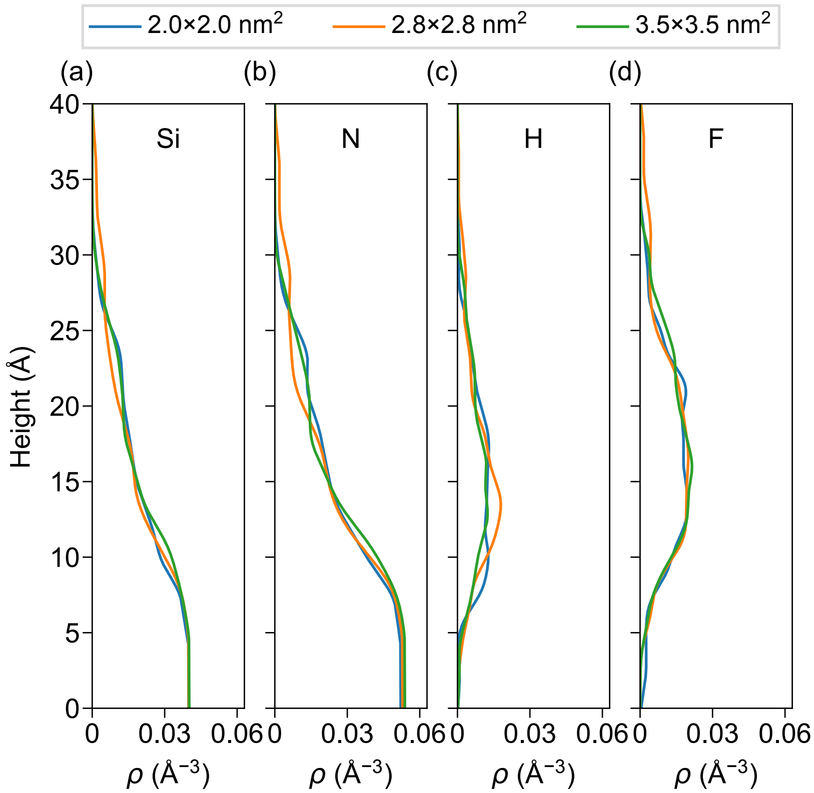

Figure S5: Atomic density profiles of surfaces after the etching simulation for areas of 2.0×2.0 nm^2, 2.8×2.8 nm^2, and 3.5×3.5 nm^2 for (a) Si, (b) N, (c) H, and (d) F.

Table S4: Desorption probabilities and reaction probabilities for Si and N surface species during steady-state etching, derived from MD simulations.

Surface species (i)	Desorption probability Γ_i ($\times 10^{-3}$ nm^2/HF)	Reaction probability r_i, q_i ($\times 10^{-3}$ nm^2/HF)
SiF_0	0.77349	20.672
SiF_1	2.3288	15.570
SiF_2	9.7272	19.934
SiF_3	54.605	-
NH_0	6.4533	8.3217
NH_1	4.8023	8.7203
NH_2	34.993	-

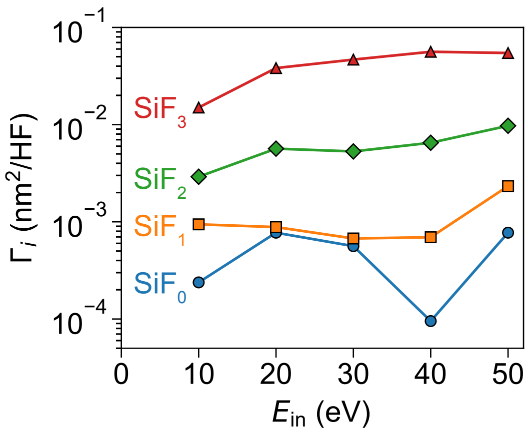

Figure S6: Desorption probabilities of Si surface species as a function of E_{in} when $\theta_{\mathrm{in}} = 0°$.