Supporting Information

Investigation on the Combustion Mechanism for NF₃/H₂ in DF/HF Chemical Lasers: A New Perspective Based on Deep Potential Molecular Dynamics Simulation

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The active learning process for NF_3/H_2 system consisted of totally 27 iterations. In each iteration, successive short MD simulations were run, and numbers of frames were selected to calculate the accuracy rate. If the accuracy rate decreased, newly generated candidate structures were added into the dataset, and the next iteration process commenced. Once the accuracy rate was stable, then the dataset was considered complete, and the neural network potential was fully trained. The details of the training process are summarized in **Table S1**.

Iteration	Time length	Number of frames	Accuracy rate	Candidate	Failed
	(ps)		(%)	(%)	(%)
1	0.01	210	100	0	0
1	0.02	410	100	0	0
1	0.05	1010	100	0	0
1	0.1	1010	88.7	11.3	0
2	0.1	1010	97.4	2.6	0
3	0.1	1010	98.8	1.2	0
3	0.2	1010	97.6	2.4	0

Table S1. Details of the Active Learning Process for the combustion of NF₃/H₂.

3	0.4	1010	97.8	2.2	0
3	0.8	1010	97.1	2.1	0
3	1.2	1210	97.3	2.7	0
3	1.6	1610	96.8	3.2	0
3	2.0	2010	96.7	3.3	0
3	2.4	2410	93.6	6.3	0.1
4	2.4	2410	92.9	3.8	4.0
5	2.4	2410	95.2	4.7	0.1
6	2.4	2410	96.0	4.0	0
7	2.4	2410	96.4	3.6	0
7	4.0	2010	95.5	4.0	0.5
8	4.0	2010	97.8	2.1	0.1
8	8.0	2010	92.0	7.7	0.3
9	8.0	2010	94.4	3.9	1.7
10	8.0	2010	95.6	4.0	0.4
10	16	2010	88.0	10.0	4.0
11	16	2010	78.6	14.0	7.4
12	16	2010	98.8	1.1	0.1
12	32	2010	97.6	2.3	0.1
12	48	2010	97.8	2.1	0.1
12	50	2010	96.7	3.2	0.1
13	50	2010	98.1	1.9	0.1
13	50.5	2010	97.1	2.8	0.1
14	50.5	2010	85.1	10.2	4.7
15	50.5	2010	31.7	2.2	66.1
16	50.5	2010	32.0	18.9	49.1
17	50.5	2010	72.7	26.9	0.4
18	50.5	2010	61.0	8.2	30.8
19	50.5	2010	88.7	11.0	0.3
20	50.5	2010	86.5	5.8	7.7
21	50.5	2010	94.2	5.7	0.1
22	50.5	2010	92.6	7.3	0.1
23	50.5	2010	67.3	15.4	17.3
24	50.5	2010	92.4	7.4	0.2
25	50.5	2010	96.2	3.7	0.1
26	50.5	2010	96.7	3.2	0.1
27	50.5	2010	97.5	2.5	0
27	101	2010	98.2	1.8	0
27	202	2010	98.5	1.5	0
27	402	2010	98.7	1.3	0
27	606	2010	98.9	1.1	0
27	808	2010	98.9	1.0	0.1
27	1010	2010	98.6	1.4	0



Fig. S1 (a) The evolution of species numbers in MD simulations at 4000 K; (b) The evolution of species numbers in MD simulations at 5000 K; (c) The evolution of NF3 numbers in MD simulations at different temperatures; (d) Final populations of NF₃, F, HF, and N₂ after thermal decomposition of NF₃/H₂ system with different temperatures.