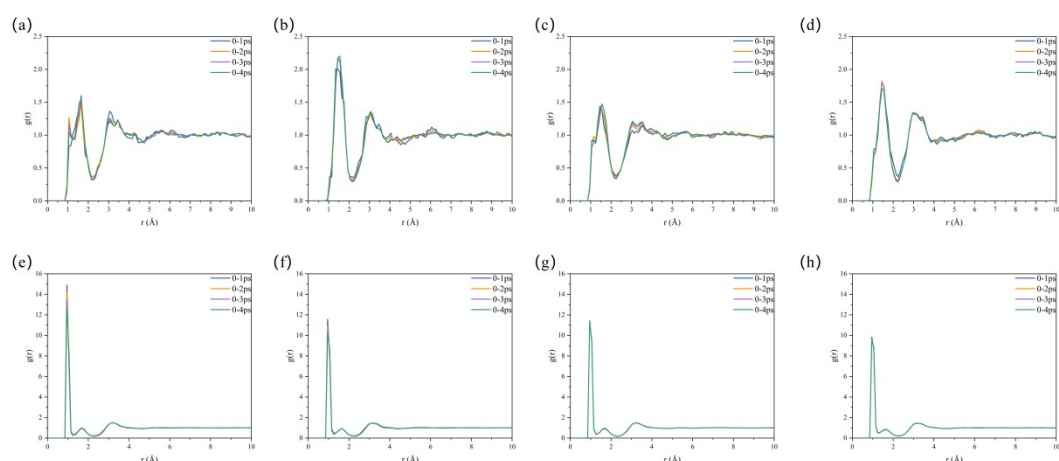


S1: RDFs at different simulation durations



S1 RDFs at different simulation durations: (a) H–F in the 353 K–23% system; (b) H–F in the 353 K–46% system; (c) H–F in the 453 K–23% system; (d) H–F in the 453 K–46% system; (e) H–O in the 353 K–23% system; (f) H–O in the 353 K–46% system; (g) H–O in the 453 K–23% system; (h) H–O in the 453 K–46% system.

S2: Peak shape information of F-H in four different systems

	353K-23%P ₂ O ₅		353K-46%P ₂ O ₅		453K-23%P ₂ O ₅		453K-46%P ₂ O ₅	
	Peak distance	g(r)	Peak distance	g(r)	Peak distance	g(r)	Peak distance	g(r)
0-1ps	1.65	1.5995	1.45	2.0093	1.45	1.4376	1.45	1.8185
0-2ps	1.65	1.4875	1.45	2.1246	1.55	1.3710	1.45	1.8275
0-3ps	1.65	1.5541	1.45	2.1754	1.55	1.3455	1.45	1.8040
0-4ps	1.65	1.5610	1.45	2.1743	1.55	1.2991	1.45	1.7083

*The initial values of bond length and bond angle are 3.5Å and 120°.

S3: Peak shape information of O-H in four different systems

	353K-23%P ₂ O ₅		353K-46%P ₂ O ₅		453K-23%P ₂ O ₅		453K-46%P ₂ O ₅	
	Peak distance	g(r)	Peak distance	g(r)	Peak distance	g(r)	Peak distance	g(r)
0-1ps	0.95	14.9147	0.95	11.5636	0.95	11.2924	0.95	9.8307
0-2ps	0.95	14.2197	0.95	10.9040	0.95	11.3858	0.95	9.6147
0-3ps	0.95	13.3899	0.95	10.3631	0.95	11.4115	0.95	9.5224
0-4ps	0.95	12.8676	0.95	10.1456	0.95	11.3522	0.95	9.5408

*The initial values of bond length and bond angle are 3.5Å and 120°.

S4: Sensitivity test of H₂O–H₃PO₄–HF system in DPMD(τ_{cont})

type	Single factor of key length (fixed key angle value)					Single factor of key angle (fixed value of key length)				
	-0.4	-0.2	0	+0.2	+0.4	-20	-10	0	+10	+20
P–O⋯H _p	1.944	1.945	1.952	1.969	1.982	2.062	2.019	1.952	1.895	1.856
P–O⋯H _w	2.238	2.218	2.237	2.300	2.359	2.290	2.279	2.237	2.236	2.334
P–O⋯H _b	1.824	1.811	1.835	1.891	1.930	1.869	1.859	1.835	1.825	1.866

H _p ···O _w	2.152	2.137	2.147	2.208	2.273	2.221	2.184	2.147	2.118	2.104
H _w ···O _w	2.492	2.460	2.477	2.540	2.609	2.669	2.578	2.477	2.488	2.641
H _h ···O _w	2.127	2.078	2.078	2.128	2.172	2.166	2.115	2.078	2.098	2.198
H _p ···F	4.908	4.776	4.599	4.415	4.251	5.445	4.940	4.599	4.268	3.929
H _w ···F	3.927	3.865	3.825	3.817	3.806	3.882	3.851	3.825	3.848	3.941
H _h ···F	2.570	2.538	2.520	2.521	2.527	2.595	2.541	2.520	2.541	2.610

*The initial values of bond length and bond angle are 3.5Å and 120°.

S5: Sensitivity test of H2O-H3PO4-HF system in DPMD(τ_{int})

type	Single factor of key length (fixed key angle value)					Single factor of key angle (fixed value of key length)				
	-0.4	-0.2	0	+0.2	+0.4	-20	-10	0	+10	+20
P-O···H _p	13.583	13.348	13.187	13.175	13.212	15.471	14.730	13.187	11.947	11.231
P-O···H _w	9.427	9.303	9.240	9.310	9.423	10.038	9.624	9.240	8.780	8.285
P-O···H _h	7.934	7.871	7.750	7.856	7.910	8.253	8.074	7.750	7.436	7.076
H _p ···O _w	17.117	16.573	16.205	16.241	16.342	17.421	16.834	16.205	15.450	14.563
H _w ···O _w	13.678	13.516	13.340	13.259	13.066	14.939	14.220	13.340	12.396	11.404
H _h ···O _w	13.443	13.110	12.781	12.572	12.322	13.521	13.221	12.781	12.368	11.899
H _p ···F	40.761	40.105	38.904	37.889	36.063	46.009	42.359	38.904	36.332	33.969
H _w ···F	27.121	26.949	26.781	26.428	25.963	28.847	28.068	26.781	25.073	23.499
H _h ···F	23.650	23.312	22.829	22.481	21.921	25.890	24.508	22.829	22.462	22.271

*The initial values of bond length and bond angle are 3.5Å and 120°.

S6: Sensitivity test of H2O-H3PO4 system in DPMD(τ_{cont})

type	Single factor of key length (fixed key angle value)					Single factor of key angle (fixed value of key length)				
	-0.4	-0.2	0	+0.2	+0.4	-20	-10	0	+10	+20
P-O···H _p	2.066	2.070	2.082	2.100	2.118	2.205	2.153	2.082	2.018	1.963
P-O···H _w	2.201	2.174	2.181	2.226	2.269	2.229	2.222	2.181	2.171	2.268
P-O···H _h	1.779	1.770	1.777	1.802	1.826	1.798	1.792	1.777	1.761	1.782
H _p ···O _w	2.324	2.300	2.288	2.306	2.335	2.354	2.320	2.288	2.266	2.243
H _w ···O _w	2.399	2.343	2.333	2.375	2.425	2.461	2.398	2.333	2.356	2.483
H _h ···O _w	2.052	2.0163	2.003	2.021	2.037	2.048	2.024	2.003	2.004	2.046

*The initial values of bond length and bond angle are 3.5Å and 120°.

S7: Sensitivity test of H2O-H3PO4 system in DPMD(τ_{int})

type	Single factor of key length (fixed key angle value)					Single factor of key angle (fixed value of key length)				
	-0.4	-0.2	0	+0.2	+0.4	-20	-10	0	+10	+20
P-O···H _p	22.375	22.242	22.289	22.382	22.603	24.557	23.596	22.289	20.996	19.907
P-O···H _w	15.581	15.407	15.504	15.580	15.804	16.347	16.0190	15.504	14.904	14.168
P-O···H _h	14.373	14.374	14.213	14.528	14.502	14.622	14.326	14.213	14.213	14.299
H _p ···O _w	26.542	26.093	25.712	25.543	25.495	26.872	26.286	25.712	25.264	24.379
H _w ···O _w	22.099	21.917	21.728	21.585	21.446	23.000	22.402	21.728	20.889	20.125
H _h ···O _w	20.459	20.077	19.785	19.693	19.631	20.630	20.224	19.785	19.314	18.773

S8: Hydrogen bond lifetime error of DPMD

	H ₂ O-H ₃ PO ₄ -HF		H ₂ O-H ₃ PO ₄	
	τ_{cont}	τ_{int}	τ_{cont}	τ_{int}
P-O...H _p	1.952 \pm 0.0041	13.187 \pm 0.0653	2.082 \pm 0.0051	22.289 \pm 0.2760
P-O...H _w	2.237 \pm 0.0080	9.240 \pm 0.0576	2.181 \pm 0.0071	15.504 \pm 0.2102
P-O...H _h	1.835 \pm 0.0067	7.750 \pm 0.0518	1.777 \pm 0.0063	14.213 \pm 0.2472
H _p ...O _w	2.147 \pm 0.0034	16.205 \pm 0.1266	2.288 \pm 0.0043	25.712 \pm 0.2945
H _w ...O _w	2.477 \pm 0.0042	13.340 \pm 0.0742	2.333 \pm 0.0042	21.728 \pm 0.2781
H _h ...O _w	2.078 \pm 0.0038	12.781 \pm 0.1006	2.003 \pm 0.0040	19.785 \pm 0.2762
H _p ...F	4.599 \pm 0.0554	38.904 \pm 0.2925	/	/
H _w ...F	3.825 \pm 0.0322	26.781 \pm 0.1148	/	/

*Unit:ps

S9 Average number of strong hydrogen bonds of H₂O-H₃PO₄-HF system

Type	Segment 1	Segment 2	Segment 3	Segment 4
P-O...H _p	248.08 \pm 67.7	640.5 \pm 70.4	674.26 \pm 58.2	657.82 \pm 45.7
P-O...H _w	649.24 \pm 398.9	246.56 \pm 52.3	304.5 \pm 30.1	318.92 \pm 26.9
P-O...H _h	197.78 \pm 81.6	98.18 \pm 17.0	133.38 \pm 18.6	137.67 \pm 22.6
H _p ...O _w	601.06 \pm 156.3	1093.26 \pm 217.5	1434.96 \pm 105.3	1596.90 \pm 71.0
H _w ...O _w	3227 \pm 1833.5	1060.14 \pm 116.9	1254.58 \pm 88.8	1365.33 \pm 81.4
H _h ...O _w	1295.92 \pm 340.3	659.8 \pm 61.7	823.6 \pm 49.4	889.02 \pm 45.9
H _p ...F	28.32 \pm 13.5	72.72 \pm 25.2	118.88 \pm 8.7	109.53 \pm 11.4
H _w ...F	347.62 \pm 91.9	236.6 \pm 127.7	75.94 \pm 9.0	72.76 \pm 7.8
H _h ...F	63.24 \pm 29.3	36.4 \pm 9.5	56.6 \pm 8.9	54.84 \pm 7.7

S10 Average number of receptor atoms of H₂O-H₃PO₄-HF system

Type	Segment 1	Segment 2	Segment 3	Segment 4
O _p	495.16 \pm 222.7	251.2 \pm 27.6	304.18 \pm 15.3	312.7647 \pm 14.5
O _w	3428.4 \pm 896.5	145.06 \pm 246.5	1223.94 \pm 36.0	1264.098 \pm 24.2
F	154.98 \pm 8.7	167.48 \pm 1.3	158.66 \pm 3.6	154.6275 \pm 1.2

S11 Average number of strong hydrogen bonds of H₂O-H₃PO₄ system

Type	Segment 1	Segment 2	Segment 3	Segment 4
P-O...H _p	447.3867 \pm 208.9	715.3333 \pm 40.1	621 \pm 44.1	635.9481 \pm 40.2
P-O...H _w	664.04 \pm 576.5	286.4533 \pm 30.5	282.7467 \pm 30.4	261.7273 \pm 34.9
P-O...H _h	175.0133 \pm 96.8	135.44 \pm 18.7	136.6933 \pm 18.6	136.026 \pm 15.7
H _p ...O _w	939 \pm 192.2	1474.6933 \pm 85.4	1577.3333 \pm 61.5	1595.0779 \pm 54.3
H _w ...O _w	2725.6667 \pm 2047.9	1186.7333 \pm 71.6	1262.8533 \pm 87.0	1281.9091 \pm 84.1
H _h ...O _w	964.5067 \pm 340.2	816.2 \pm 62.6	925.3733 \pm 42.9	978.026 \pm 49.8

S12 Average number of receptor atoms of H₂O-H₃PO₄ system

Type	Segment 1	Segment 2	Segment 3	Segment 4
O _p	507.76 \pm 277.6	337.2133 \pm 14.1	341.1333 \pm 20.6	359.8831 \pm 13.7

O _w	2867.4533±1250.3	1176.92±63.1	1208.8133±30.2	1185.7403±31.5
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