Supporting Information

The local hydrogen bonding environment promotes the deprotonation of surface hydroxyl groups for continuing ammonia decomposition

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S1. DFT+U

DFT+U and DFT calculations for NH_3 mediated PT, a Hubbard U = 5.4 eV correction was applied to the 3d orbitals of Ti based on Mulliken population analysis.

Table S1. DFT+U and DFT calculation results of NH_3 mediated PT

NH_3 mediated PT		O charge (e)	H charge (e)	OH length (Å)	H-bond length (Å)	Ea (eV)
DFT+U	only NH_3	-0.598	0.144	0.989	1.938	0.355
	neighbour NH_3	-0.606	0.146	0.988	1.911	0.357
	neighbour H_2O	-0.614	0.153	0.994	1.863	0.284
DFT	only NH_3	-0.489	0.134	0.987	1.945	0.354
	neighbour NH_3	-0.505	0.139	0.984	1.971	0.401
	neighbour H_2O	-0.521	0.144	0.993	1.858	0.314

S2.The a-TiO_2(101) slab model

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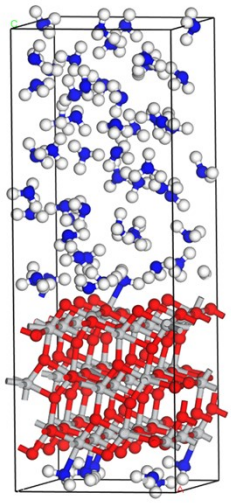
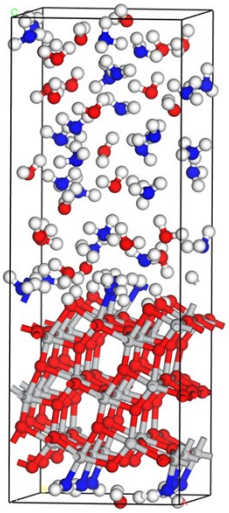


non-hydroxylated a-TiO_2(101) slab model including 60 NH_3 molecules

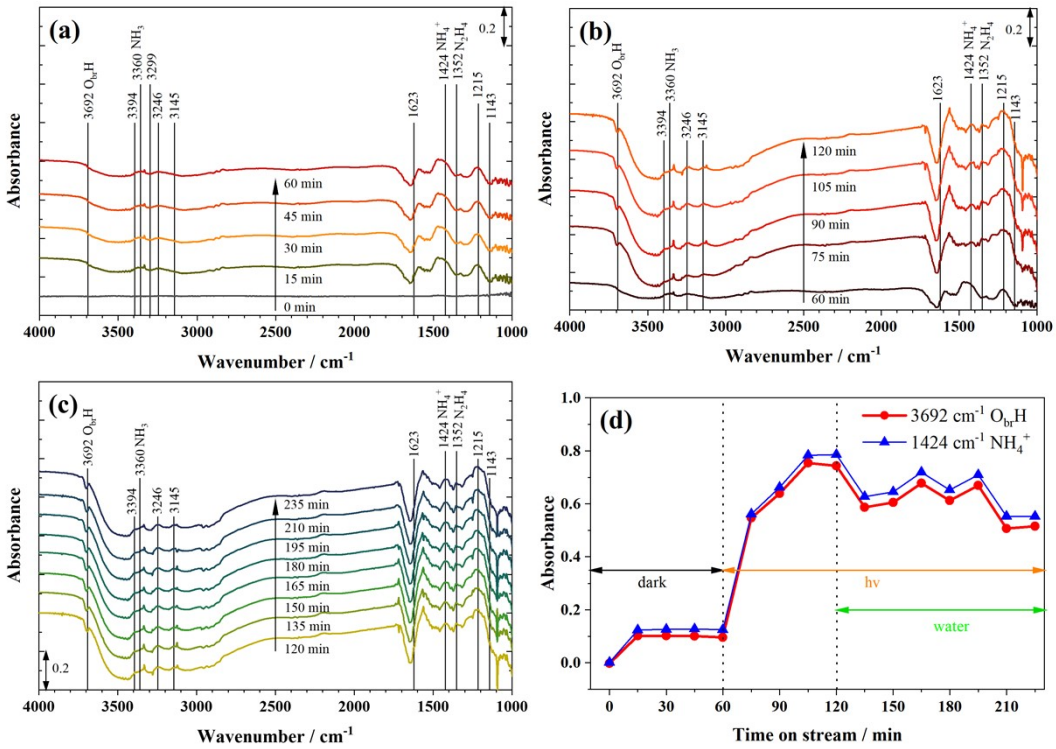


hydroxylated a-TiO_2(101) slab model including 36 NH_3 molecules and 24 H_2O molecules

FPMD simulation was performed in a long relaxation time (~30 ps) to obtain well relaxated configurations of ammonia and water molecules before sampling.

S3. Experiment

Anatase TiO_2 sample with loading of about 0.1 wt % Pt was prepared by photodeposition method. The TiO_2 powder was dispersed into an aqueous ethanol solution of the metal precursors, stirred vigorously in a beaker, and then light irradiated under a 300 W Xe lamp for 3 h. The powders were then filtered by aspiration, washed with ethanol and water, and dried at 323 K overnight. The in-situ diffuse reflectance infrared Fourier transform spectra (DRIFTS) were performed by Bruke Tensor Ⅱ FTIR NEXUS spectrometer. The sample was heated at 473 K for 90 min under flowing He and photo irradiation for surface clean-up. In dark condition, ammonia (1 mL/min) carried by He gas (20 mL/min) was introduced into the reaction cell until the adsorption reached equilibrium after 60 min. Later, the Xe lamp was turned on to driven the photocatalytic decomposition reaction and the spectrum was taken. After 60 min, water vapor (0.5 ml /min) carried by He gas (20 mL/min) was introduced into the cell, and the test was finished after 120 min.



In-situ DRIFTS spectra results of the Pt/TiO_2 sample under the flow of ammonia vapor. (a) In the dark from 0 to 60 min. (b) Under photoirradiation from 60 to 120 min. (c) Under photoirradiation with flowing water vapor from 120 to 235 min. (d) The time course of the band intensity at 3692 cm^{-1} and 1424 cm^{-1} during these procedures.

S4. Definition of H-bonds occupancy

$$Occupancy = N_{H\text{-}bonds} / N_{total}$$

Where $N_{H\text{-}bonds}$ is number of frames with hydrogen bonds exist along FPMD trajectory, N_{total} is number of total frames.

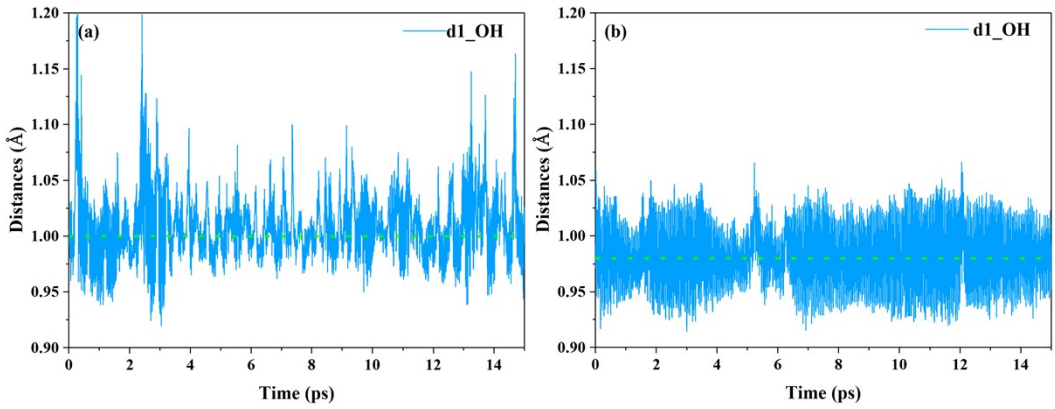


Figure S1. Time evolution of OH bond length of surface hydroxyl group for (a) ammonia-water mixture and (b) pure ammonia. The green dashed line is the average bond length.

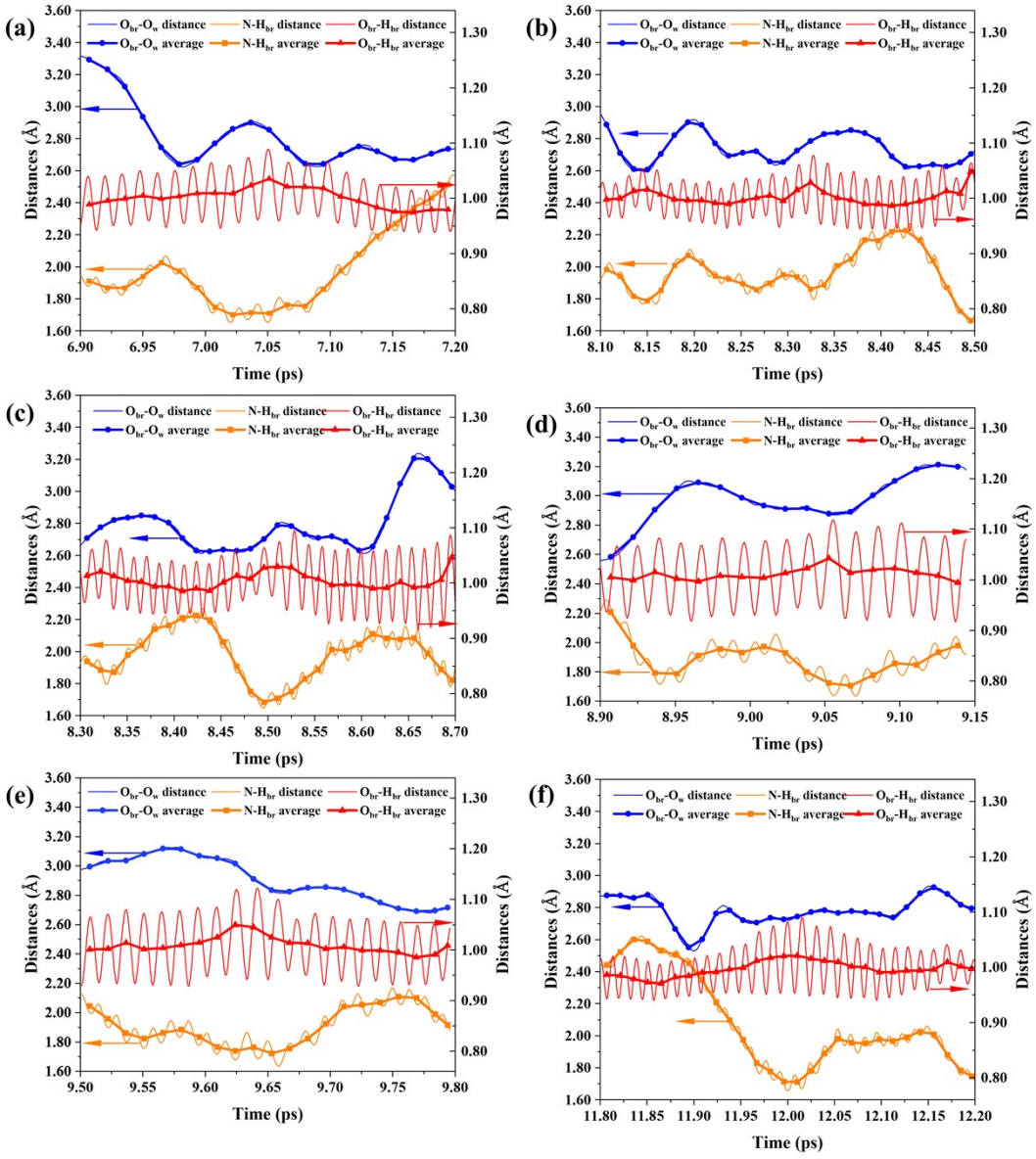
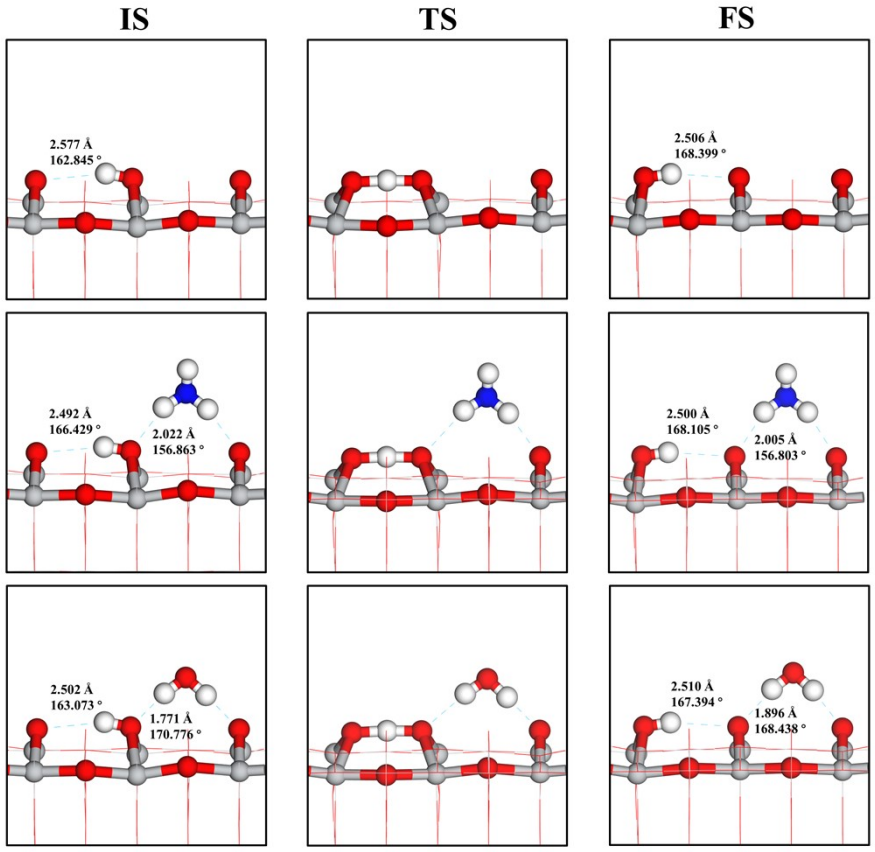


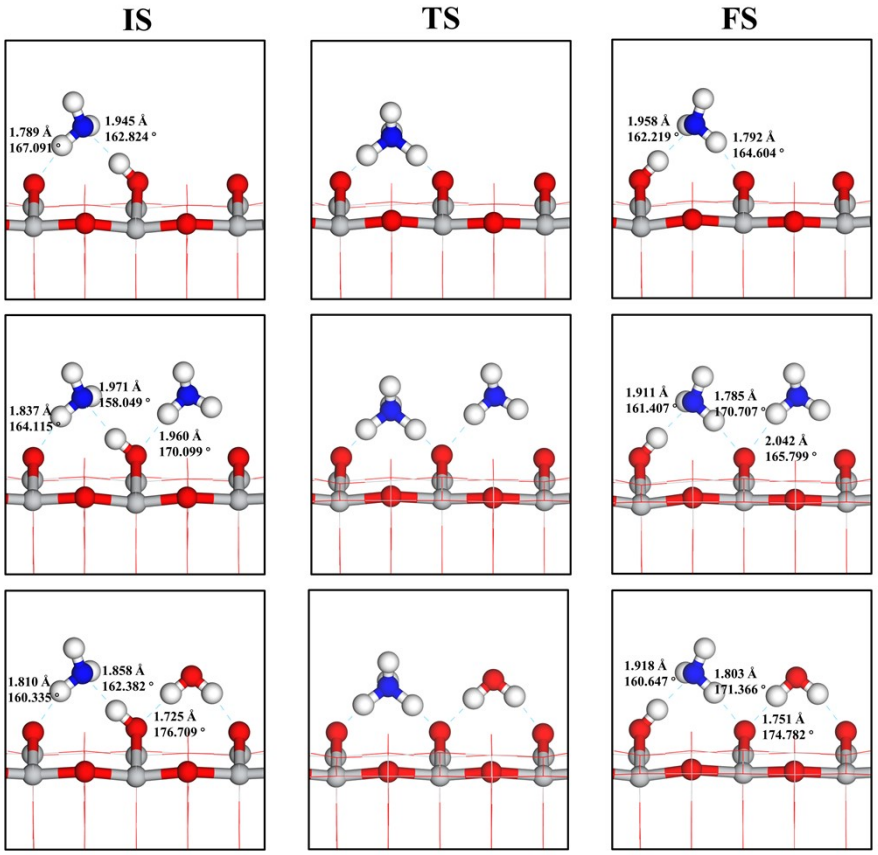
Figure S2. Time evolution of O_{br}-O_w, N-H_{br}, O_{br}-H_{br} distances, and its average distances, at about (a) 7.05 ps, (b) 8.33 ps, (c) 8.53 ps, (d) 9.05 ps, (e) 9.62 ps, (f) 12.02 ps.

As the O_{br}-O_w distances reduces, the O_{br}-H_{br} bond lengths increases, and the O_{br}-O_w distances reduction are not strictly always reduced (there may be some fluctuations, but the overall effects are on a downward trend over longer time interval). Generally, when the O_{br}-O_w distances are less than 3.0 Å, the increase in the Obr-Hbr bond lengths is more pronounced due to the reduction of the O_{br}-O_w distances.

(a) direct PT



(b) NH_3 mediated PT



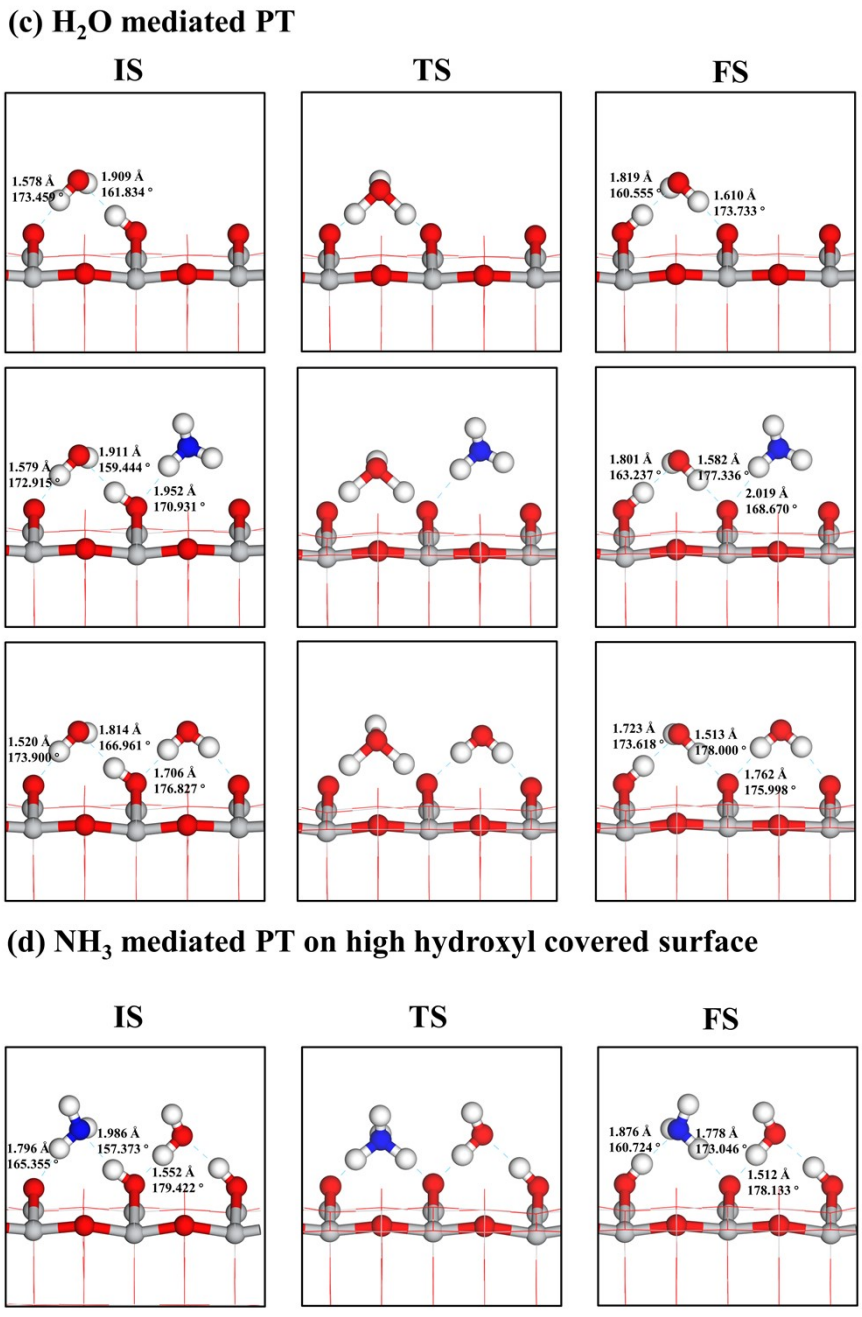


Figure S3. Initial state (IS), transitional state (TS) and final state (FS) adsorption configuration of (a) direct PT, (b) NH_3-mediated PT and (c) H_2O-mediated PT with existence of neighbouring H_2O molecule; (d) NH_3-mediated PT with existence of neighbouring H_2O molecule on high hydroxyl covered surface. The bond length values and bond angle values of H-bonds associated with $O_{br}H$ deprotonation are marked out.

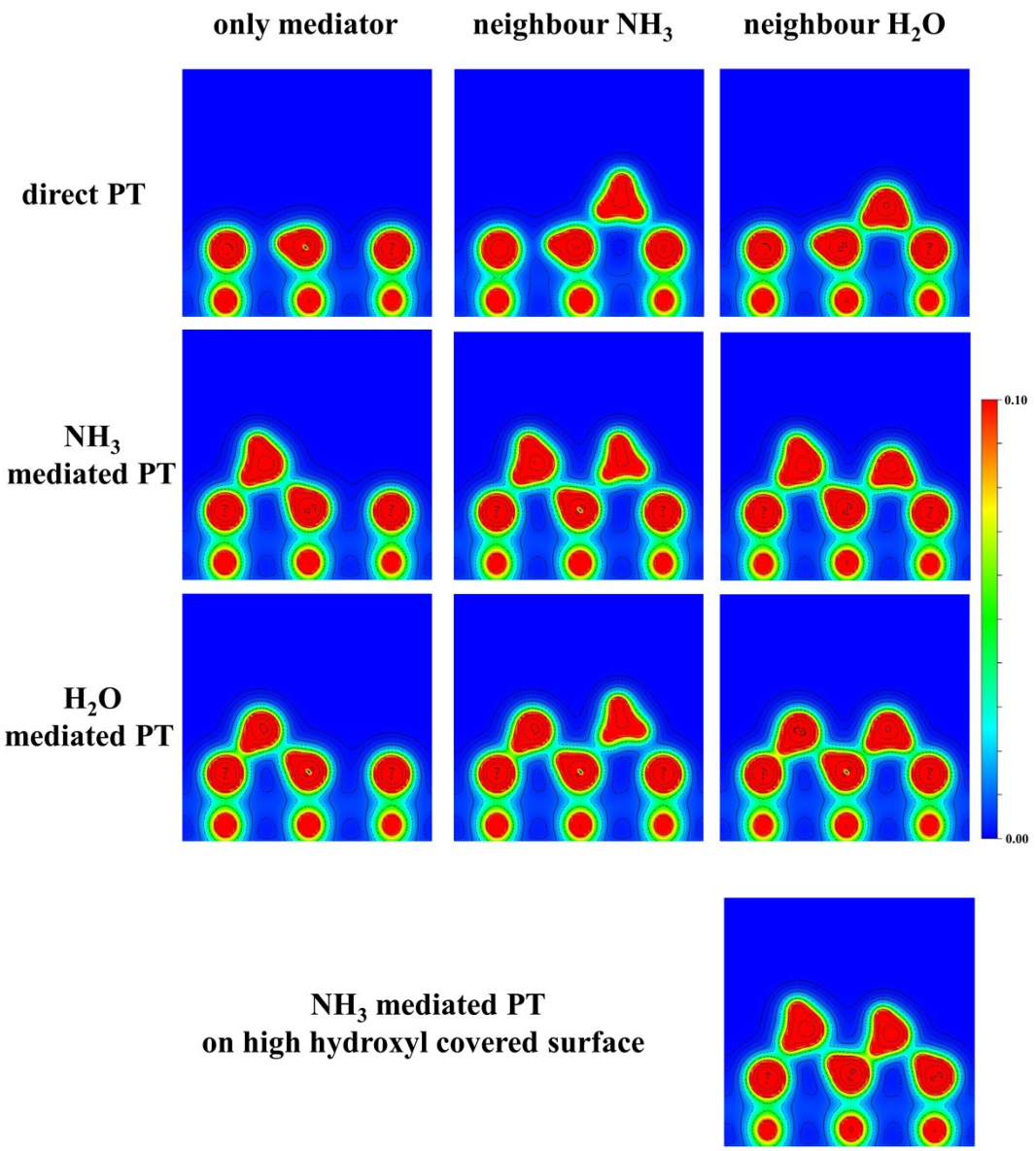


Figure S4. Electron density contour map of initial state configuration.

As shown in Figure S4, there is an electron sharing density of local H-bonds involving $O_{br}H$ groups in NH_3 and H_2O mediated PT. While the H-bonds of $O_{br}H$ groups in direct PT have a lower electron sharing density.

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N	8.74838600E+00	1.07470010E+01	6.54563000E-01
N	3.21712000E+00	1.54488500E+00	1.03688200E+00
N	5.21391700E+00	9.19527100E+00	2.34692120E+01
N	5.14988200E+00	3.60324800E+00	1.61324530E+01
N	1.76566500E+00	7.68860300E+00	2.16473830E+01
N	7.41663000E+00	5.02036300E+00	1.45263590E+01
N	7.03890900E+00	5.84642300E+00	2.12403410E+01
N	6.04616000E+00	2.63515700E+00	2.59444260E+01
N	1.04090010E+01	4.38299200E+00	2.10922990E+01
N	8.90837000E-01	1.29630200E+00	2.82050830E+01
N	7.00804200E+00	5.40755300E+00	2.71717320E+01
N	3.49219800E+00	9.37015700E+00	1.48448110E+01
N	4.91697200E+00	6.69267600E+00	2.54791090E+01
N	5.70380400E+00	2.09567000E-01	2.81359180E+01
N	3.26797100E+00	4.09813200E+00	2.25727190E+01
N	8.08554200E+00	2.12669800E+00	1.87713080E+01
N	6.61525400E+00	9.89048000E+00	1.84201860E+01
N	1.03653690E+01	8.51078500E+00	2.83425290E+01
N	2.31550600E+00	5.01055200E+00	1.90903480E+01
N	6.58140000E-02	7.55010900E+00	1.52783420E+01
N	1.02610510E+01	2.99873300E+00	2.48015890E+01
N	3.69225400E+00	2.11939700E+00	2.07002680E+01
N	1.02788380E+01	1.01119120E+01	2.49143130E+01
N	8.56957000E+00	1.48944200E+00	2.22533840E+01
N	2.32555100E+00	1.08614240E+01	1.83271820E+01
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H	6.36016100E+00	2.70429000E+00	1.27357280E+01
H	6.22770000E-01	8.72149200E+00	1.36825500E+01
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H	6.94254200E+00	1.67129000E-01	1.23492890E+01
H	5.24520000E-01	6.25745700E+00	1.32652070E+01
H	6.14660700E+00	4.17833100E+00	1.33117090E+01
H	4.72821500E+00	6.66928900E+00	1.34847680E+01
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H	5.90605800E+00	3.19313000E-01	1.35904280E+01
H	9.99340000E-01	4.09665000E-01	1.30226890E+01
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H	9.81626000E+00	3.28416400E+00	1.03010000E-02
H	8.20492800E+00	3.71698700E+00	3.19924000E-01
H	3.00869300E+00	6.33411900E+00	4.36179000E-01
H	2.63756300E+00	2.35212200E+00	8.90018000E-01
H	3.90675000E+00	9.76213900E+00	3.07268000E-01
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H	8.23391100E+00	7.48976000E+00	4.02038000E-01
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H	3.37752100E+00	1.01301650E+01	1.26283020E+01
H	8.15397200E+00	7.91391300E+00	1.18204000E+01
H	8.06911500E+00	5.12885400E+00	1.27569190E+01
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H	6.08769900E+00	8.69206000E+00	2.35904710E+01

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  &END COORD
  &KIND Ti
    BASIS_SET DZVP-MOLOPT-SR-GTH
    POTENTIAL GTH-PBE-q12
    &END KIND
    &KIND O
    BASIS_SET DZVP-MOLOPT-SR-GTH
    POTENTIAL GTH-PBE-q6
    &END KIND
    &KIND N
    BASIS_SET DZVP-MOLOPT-SR-GTH
    POTENTIAL GTH-PBE-q5
    &END KIND
    &KIND H
    MASS 2.014102
    BASIS_SET DZVP-MOLOPT-SR-GTH
    POTENTIAL GTH-PBE-q1
    &END KIND
  &END SUBSYS
&END FORCE_EVAL
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Snapshoot coordinates at 9.620 ps for ammonia-water mixture

Ti	2.0916895094	9.6197414055	3.9850537452	O	6.2184432081	7.6330668261	2.5794629307
Ti	2.0818731849	1.9904838356	4.0277911789	O	7.6226963165	0.0657964028	6.0820109540
Ti	2.1055194741	5.7393833375	4.0667824008	O	7.6876179276	3.8505292632	6.1469222251
Ti	3.4725857015	9.5473846746	7.5588735634	O	7.6243980877	7.4793936948	6.2565853670
Ti	3.5276781816	1.8681857417	7.4548228011	O	9.0824772442	-0.0110348223	9.8054430656
Ti	3.5199335545	5.6133841546	7.5573474026	O	9.0805140985	3.9966259151	9.7446054539
Ti	4.9287099032	9.6867095215	11.2012857449	O	9.0740417291	7.7531904214	9.7660406769
Ti	4.9292501887	2.0211276970	11.0675749042	O	3.9712355544	9.6161810248	3.3151422026
Ti	4.9691661006	5.7754817792	11.1108781175	O	3.9206106095	1.8511613201	3.2402809085
Ti	7.3866096126	0.0285631691	4.0687470722	O	4.0538941534	5.7600161456	3.2744934154
Ti	7.4629882310	3.8866135973	3.9136262669	O	5.2637160304	9.5466586243	6.9875229993
Ti	7.3998628100	7.6597255921	4.0151689234	O	5.4058406971	1.8693025508	6.9272619905
Ti	8.7803883852	0.0737272489	7.6428305059	O	5.4547896122	5.7082267932	6.9953620946
Ti	8.7663623214	3.9080686913	7.6683155460	O	6.7634379611	9.6834625073	10.7348943152
Ti	8.6874162793	7.6216604291	7.6646415551	O	6.9024958469	1.9103528852	10.6575630849
Ti	10.2656669712	0.0064566328	11.2167799201	O	6.9381716472	5.7256244471	10.7098987609
Ti	10.2784264743	3.8815610659	11.0888902100	O	9.2150388246	0.1281331056	3.3140443765
Ti	10.0591763888	7.7429576549	11.2572905112	O	9.1505456731	3.9846901202	2.9904901315
Ti	9.5595430213	9.5969382621	2.9664024881	O	9.3123504799	7.6434395517	3.2489079885
Ti	0.4808649004	9.5500212756	6.5932370876	O	10.4903743304	0.0008426121	6.9607868648
Ti	9.6007601835	2.0053382670	2.9442343480	O	1.6343086941	0.1093516041	10.5156591359
Ti	0.4507274069	2.0502109266	6.5430860403	O	0.1239085667	3.9159885303	6.8642161519
Ti	9.7501378377	5.8771033808	2.8041478846	O	1.6774066757	4.0037777742	10.3612254509
Ti	0.5503305061	5.8217507942	6.5883252346	O	10.5284314493	7.6124583571	7.0561366215
Ti	1.9441810617	9.5911139964	10.1606166217	O	1.5894631465	7.7930967657	10.5564249126
Ti	1.9411240380	1.9058071652	10.2016424193	O	4.8776677245	0.1721920336	16.9712236816
Ti	1.9372347602	5.8739134857	10.2063754982	O	1.6929663100	4.8149971954	24.3904128376
Ti	4.5131144783	0.0460980386	2.9597412758	O	-1.2183571378	2.7861636568	15.7321883170
Ti	4.3125437687	3.8006406526	3.0621496632	O	4.1195572888	-0.7258510344	21.8022209639
Ti	4.3749242059	7.6880784597	3.1237294150	O	1.5525891155	3.6943916213	20.2418219310
Ti	5.7745435431	0.0315757474	6.5917294594	O	3.6829250547	5.2587832522	21.0186398585
Ti	5.7765032574	3.8298826766	6.5605969278	O	7.5745283685	8.3424081242	27.5936217028
Ti	5.6861422665	7.6059083713	6.7526334762	O	2.8400968946	1.6131183941	15.5071508314
Ti	7.2814429019	0.0802994205	10.2495649115	O	7.5976127439	0.4361133053	16.2520697449
Ti	7.1849554406	3.8538925407	10.2374797714	O	9.0162324485	9.8472739438	14.4434076662
Ti	7.1103356579	7.6788153751	10.4025385104	O	0.0710899453	7.6566620302	23.9916020955
O	10.5380598759	9.7677152056	4.8654187034	O	5.9355996497	7.0506597124	29.4150228172
O	1.5782142788	9.6456660506	8.5031353195	O	1.5790220601	9.3697714752	25.9036898627
O	0.0634149906	1.9646378403	4.8000693799	O	10.0188437197	8.8023767744	19.7148083666
O	1.5122120367	1.9421031668	8.4206149636	O	11.8725187104	3.3288490896	26.6957449779
O	0.2445472337	5.8557278743	4.7743220203	O	3.8792795495	4.1223123451	15.1202372213
O	1.5499056142	5.7564537998	8.4695683686	O	5.7619745269	8.9349725171	17.6360887544
O	3.0336946171	9.6840799377	12.2465515104	O	8.1138378350	6.6645669438	25.2475706134
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