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Alignment Energy Change in Ammonia Formation

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Abstract: *The alignment energy change supports the non-catalysed synthesis of ammonia from atmospheric air and water.*

Keywords: *Alignment energy, ammonia formation*

1. Introduction

In this fragment we will discuss the change in alignment energy [1] during ammonia formation from atmospheric air and water with the help of nitrogen plasma [2].

2. The Formation of Ammonia from Atmospheric Air and Water

The formation of ammonia from atmospheric air and water with the help of nitrogen plasma [2] goes through three phases (1), (2), (3) as follows:

$$N_{plasma\ gas\ phase} + H_2O_{water\ phase} \xrightarrow[P/L\ interface\ reaction]{} NH_{water\ phase} + OH. \quad (1)$$

$$NH + H_2O_{water\ phase} \xrightarrow[at\ water\ phase]{} NH_2 + OH. \quad (2)$$

$$NH_2 + H_2O_{water\ phase} \xrightarrow[at\ water\ phase]{} NH_3 + OH. \quad (3)$$

First phase of ammonia formation takes place in the plasma/liquid (P/L) interface on water surface; second and third phase take place at water under the plasma/liquid interface (See Figure 1) [2].

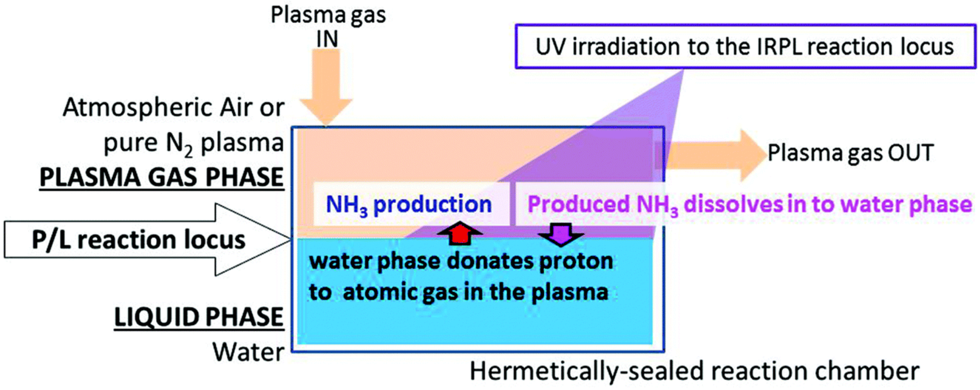

Figure 1. [2] Construction of the interfacial reaction locus between a plasma phase and a liquid phase (P/L reaction locus) for ammonia synthesis. Plasma gas sweeps across the surface of the water phase giving the reaction locus. The reaction locus is treated with UV irradiation.

Produced NH_3 dissolves in to water phase. With the help of UV irradiation to the IRPL reaction locus more ammonia is produced. The reaction can be provided at 25 °C and atmospheric pressure.

3. Alignment Characteristics of Ammonia and its Constituents

The alignment energy enables the electron to internalize its physicochemical characteristics [1]. The alignment characteristics of ammonia NH_3 and related constituents H, H_2, N, N_2, NH, NH_2 as well as water H_2O and related constituents O, O_2, OH including electron itself (e-) are presented in Table 1. Masses of the elements (H, N, O) and e- are taken from reference [3] and [4], respectively.

Table1. *The alignment characteristics of H, H_2, N, N_2, NH, NH_2, NH_3, O, O_2, OH, H_2O and e^-*

$Particle$	$Mass\ (Da)$	$R_{unaligned} = \frac{m_{particle}}{m_{e^-}} s(1)$	$n \in \mathbb{N}$	$R_{aligned} = s(n) = n\left(2 - \frac{1}{\sqrt{1+\frac{\pi^2}{n^2}}}\right)$	$W_{alignment} = \left(\frac{R_{unaligned}}{R_{aligned}} - 1\right) m_{electron} c^2$
H	1,007825031898	3117,07031	3117	3117,00158	11,2671 eV
H_2	2,015650063796	6234,14062	6234	6234,00079	11,4617 eV
N	14,003074004251	43309,66671	43309	43309,00011	**7,8651 eV**
N_2	28,006148008502	86619,33341	86619	86619,00006	1,9666 eV
NH	15,010899036149	46426,73702	46426	46426,00011	**8,1110 eV**
NH_2	30,021798072298	92853,47403	92853	92853,00005	**2,6085 eV**
NH_3	31,029623104196	95970,54434	95970	95970,00005	**2,8981 eV**
O	15,994914619257	49470,16783	49470	49470,00010	1,7326 eV
O_2	31,989829238514	98940,33567	98940	98940,00005	1,7334 eV
OH	17,002739651155	52587,23814	52587	52587,00009	**2,3132 eV**
H_2O	18,010564683053	55704,30845	55704	55704,00009	**2,8288 eV**
e-	0,00054857990907	s(1)=1,69668…	1	s(1)	0 eV

The alignment energies $W_{alignment}$ of concerned physicochemical entities are expressed in electron volts and presented in the last column of Table 1.

4. Alignment Energy Change in Ammonia Formation from Atmospheric Air and Water

We can see from Table 1 that in all three phases of ammonia formation the alignment energy is released due to accompanied water decomposition (1), (2), (3):

$$\Delta W_{H_2O \to OH} = W_{OH} - W_{H_2O} = 2{,}3132\ \text{eV} - 2{,}8288\ \text{eV} = -0{,}5156\ \text{eV}. \quad (4)$$

First phase

In the first phase the alignment energy is invested due to N → NH reaction:

$$\Delta W_{N \to NH} = W_{NH} - W_N = 8{,}1110\ eV - 7{,}8651\ \text{eV} = 0{,}2459\ \text{eV}. \quad (4a)$$

So, in the first phase only the next total alignment energy is released:

$$\Delta W_{first\ phase} = \Delta W_{H_2O \to OH} + \Delta W_{N \to NH} = -0{,}5156\ \text{eV} + 0{,}2459\ \text{eV} = -0{,}2697\ \text{eV}. \quad (4b)$$

Second phase

In the second phase the alignment energy is released due to NH → NH_2 reaction:

$$\Delta W_{NH \to NH_2} = W_{NH_2} - W_{NH} = 2{,}6085\ eV - 8{,}1110\ \text{eV} = -5{,}5025\ \text{eV}. \quad (4c)$$

So, in the second phase the next total alignment energy is released:

$$\Delta W_{second\ phase} = \Delta W_{H_2O \to OH} + \Delta W_{NH \to NH_2} = -0{,}5156\ \text{eV} - 5{,}5025\ \text{eV} = -6{,}0181\ \text{eV}. \quad (4d)$$

Third phase

In the third phase the alignment energy is invested due to NH_2 → NH_3 reaction:

$$\Delta W_{NH_2 \to NH_3} = W_{NH_3} - W_{NH_2} = 2{,}8981\ eV - 2{,}6085\ eV = 0{,}2897\ \text{eV}. \quad (4e)$$

So, in the third phase the next total alignment energy is released:

$$\Delta W_{third\ phase} = \Delta W_{H_2O \to OH} + \Delta W_{NH_2 \to NH_3} = -0{,}5156\ \text{eV} + 0{,}2897\ \text{eV} = -0{,}2259\ \text{eV}. \quad (4f)$$

5. Conclusion

In all phases of ammonia formation from water (4b), (4d), (4f) the alignment energy is released (-0,2697 eV, -6,0181 eV, -0,2259 eV) what enables the ammonia formation (1), (2), (3) without any obstacle from the alignment energy address.

Dedication

To climbing the ladder

Figure1. *Climbing the ladder [5]*

References

[1] Janez Špringer (2022) "Alignment Energy Role in Water Formation". International Journal of Advanced Research in Physical Science (IJARPS) 9(1), pp.5-8, 2022.

[2] Haruyama, Tetsuya & Namise, Takamitsu & Shimoshimizu, Naoya & Uemura, Shintaro & Takatsuji, Yoshiyuki & Hino, Mutsuki & Yamasaki, Ryota & Kamachi, Toshi & Kohno, Masahiro. (2016). Non-catalyzed One-step Synthesis of Ammonia from Atmospheric Air and Water. Green Chem.. 18. 10.1039/C6GC01560C.

[3] Meng Wang et al. The Ame2020 atomic mass evaluation. Chinese Physics C Vol. 45, No. 3 (2021) 030003

[4] CODATA, retrieved January 2022

[5] https://www.scmref.nl/low-charge-ammonia-climbing-the-ladder/

Addendum

Let us repeat the exercise in the case of heavy water:

The alignment characteristics of ammonia formed from heavy water ND_3 and related constituents D, D_2, N, N_2, ND, ND_2 as well as heavy water D_2O and related constituents O, O_2, OD including electron itself (e-) are presented in Table 2. Again, masses of the elements (D, N, O) and e- are taken from reference [3] and [4], respectively.

Table2. *The alignment characteristics of D, D_2, N, N_2, ND, ND_2, ND_3, O, O_2, OD, D_2O and e^-*

$Particle$	$Mass\ (Da)$	$R_{unaligned} = \frac{m_{particle}}{m_{e^-}} s(1)$	$n \in \mathbb{N}$	$R_{aligned} = s(n) = n\left(2 - \frac{1}{\sqrt{1+\frac{\pi^2}{n^2}}}\right)$	$W_{alignment} = \left(\frac{R_{unaligned}}{R_{aligned}} - 1\right) m_{electron} c^2$
D	2,014101777844	6229,35198	6229	6229,00079	28,8095 eV
D_2	15,994914619257	6234,14062	6234	6234,00079	28,8582 eV
N	14,003074004251	43309,66671	43309	43309,00011	**7,8651 eV**
N_2	28,006148008502	86619,33341	86619	86619,00006	1,9666 eV
ND	16,017175782095	49539,01868	49539	49539,00010	**0,1917 eV**
ND_2	18,031277559939	55768,37066	55768	55768,00009	**3,3955 eV**
ND_3	20,045379337783	61997,72263	61997	61997,00008	**5,9555 eV**
O	15,994914619257	49470,16783	49470	49470,00010	1,7326 eV
O_2	31,989829238514	98940,33567	98940	98940,00005	1,7334 eV

OD	18,009016397101	55699,51981	55699	55699,00009	**4,7681 eV**
D_2O	20,023118174945	61928,87178	61928	61928,00008	**7,1929 eV**
e-	0,00054857990907	s(1)=1,69668…	1	s(1)	0 eV

The alignment energies $W_{alignment}$ of concerned physicochemical entities are presented in the last column of Table 2.

We can see from Table 2 that in all three phases of ammonia formation the alignment energy is released duo to accompanied heavy water decomposition (1), (2), (3):

$$\Delta W_{D_2O\rightarrow OD} = W_{OD} - W_{D_2O} = 4{,}7681 \text{ eV} - 7{,}1929 \text{ eV} = -2{,}4248 \text{ eV}. \quad (5)$$

First phase

In the first phase the alignment energy is released due to N → ND composition:

$$\Delta W_{N\rightarrow ND} = W_{ND} - W_N = 0{,}1917\ eV - 7{,}8651 \text{ eV} = -\ 7{,}6734 \text{ eV}. \quad (5a)$$

So in the first phase the next total alignment energy is released:

$$\Delta W_{first\ phase} = \Delta W_{D_2O\rightarrow OD} + \Delta W_{N\rightarrow ND} = -2{,}4248 \text{ eV} - 7{,}6734 \text{ eV} = -10{,}0982 \text{ eV}. \quad (5b)$$

Second phase

In the second phase the alignment energy is invested due to ND → ND_2 composition:

$$\Delta W_{ND\rightarrow ND_2} = W_{ND_2} - W_{ND} = 3{,}3955\ eV\ - 0{,}1917 \text{ eV} = 3{,}2038 \text{ eV}. \quad (5c)$$

So in the second phase the next total alignment energy is invested:

$$\Delta W_{second\ phase} = \Delta W_{D_2O\rightarrow OD} + \Delta W_{ND\rightarrow ND_2} = -2{,}4248 \text{ eV} + 3{,}2038 \text{ eV} = 0{,}7790 \text{ eV}. \quad (5d)$$

Third phase

In the third phase the alignment energy is invested due to NH_2 → NH_3 composition:

$$\Delta W_{ND_2\rightarrow ND_3} = W_{ND_3} - W_{ND_2} = 5{,}9555\ eV - \ 3{,}3955\ eV\ =\ 2{,}5600 \text{ eV}. \quad (5e)$$

So in the third phase the next total alignment energy is invested:

$$\Delta W_{third\ phase} = \Delta W_{D_2O\rightarrow OD} + \Delta W_{ND_2\rightarrow ND_3} = -2{,}4248 \text{ eV} + 2{,}5600 \text{ eV} = 0{,}1352 \text{ eV}. \quad (5f)$$

Only in the first phase of ammonia formation from heavy water (5b) the alignment energy is released ($-10{,}0982$ eV) what supports the ammonia formation (1), (2), (3). In the other two phases (5d), (5f) some activation energy is needed ($+0{,}7790$ eV, $+0{,}1352$ eV) what could slow down the ammonia formation (2), (3) from heavy water as noted in reference [2] where the ammonia production rate in the case of D2O was less than half of that in the case of H2O.

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