Electronic Supplementary Material (ESI) for RSC Advances.

Supporting files

Green route for ammonium nitrate synthesis: Fertilizer for plant growth enhancement

Figure S1: OES spectra of the system

Figure S2: Depiction of radish sprouts after 2 days of imbibition, circled are commercial N-fertilizer.

Figure S3: Depiction of tomato after 3 days of imbibition, circled are commercial N-fertilizer.

Figure S4: Standard curve for NH_4^+, NO_2^- and $NO_2^- + NO_3^-$

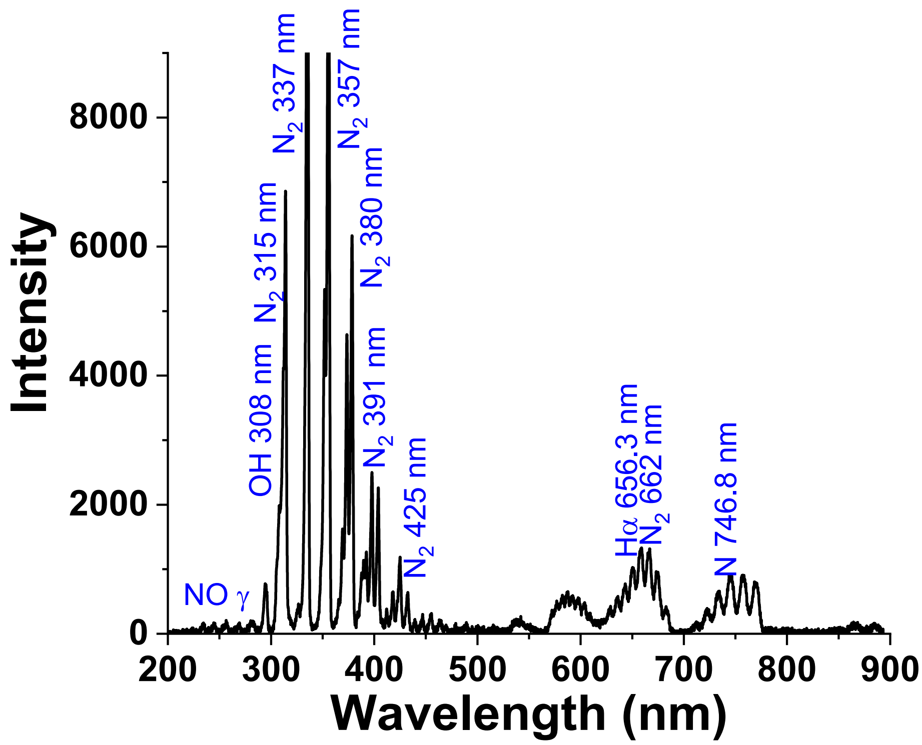

Figure S1

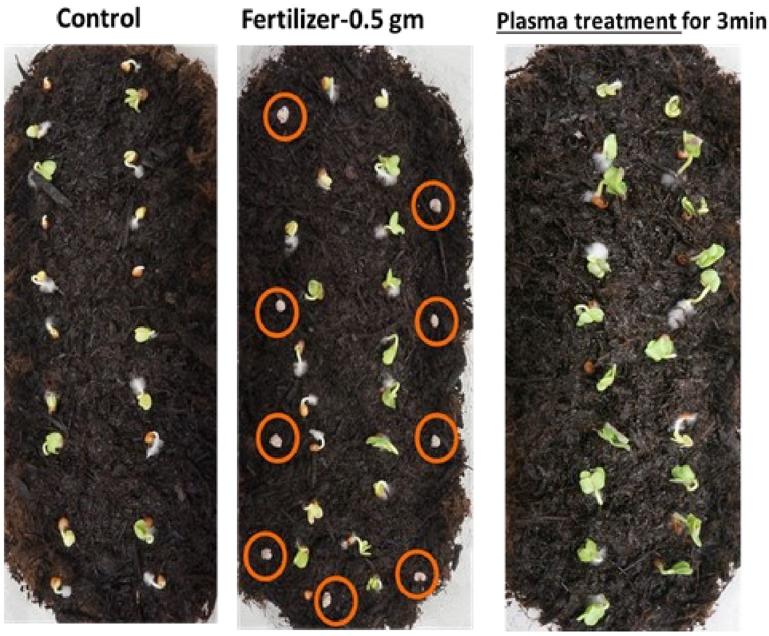

Figure S2

Figure S3

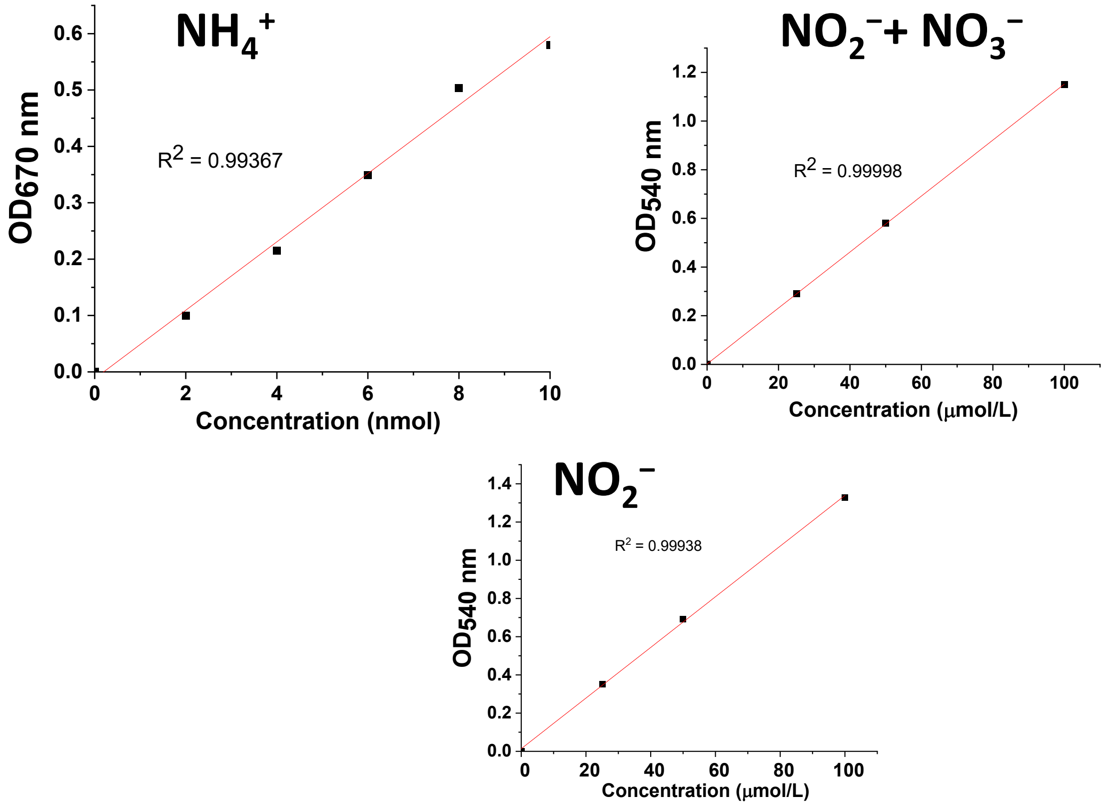
NH4+
R2 = 0.99367
OD670 nm
Concentration (nmol)
NO2−+ NO3−
R2 = 0.99998
OD540 nm
Concentration (μmol/L)
NO2−
R2 = 0.99938
OD540 nm
Concentration (μmol/L)

Figure S4

Table S1: Reactions used in the 1D-simulation.

Reactions			Ref.
$N_2 + e$	$\longrightarrow$	$2N + e$	[1,2]
$N + e$	$\longrightarrow$	$N^+ + 2e$	[1,3]
$H_2O + e$	$\longrightarrow$	$OH + H + e$	[4]
$H + e$	$\longrightarrow$	$H^+ + 2e$	[1,5]
$H_2 + e$	$\longrightarrow$	$H^+ + H + 2e$	[1,5]
$H_2 + e$	$\longrightarrow$	$H_2^+ + 2e$	[1,5]
$NH + e$	$\longrightarrow$	$NH^+ + 2e$	[1,6]
$NH + e$	$\longrightarrow$	$N^+ + H + e$	[1,6]
$NH_2 + e$	$\longrightarrow$	$NH_2^+ + 2e$	[1,6]
$NH_2 + e$	$\longrightarrow$	$NH^+ + H + 2e$	[1,6]
$NH_3 + e$	$\longrightarrow$	$NH_3^+ + 2e$	[1,6]
$NH_3 + e$	$\longrightarrow$	$NH_2^+ + H + 2e$	[1,6]
$NH + e$	$\longrightarrow$	$N + H + e$	[1,7]
$NH_2 + e$	$\longrightarrow$	$N + H_2 + e$	[1,8]
$NH_2 + e$	$\longrightarrow$	$NH + H + e$	[1,9]
$NH_3 + e$	$\longrightarrow$	$NH_2 + H + e$	[1]
$N_2 + e$	$\longrightarrow$	$N + N + e$	[1]
$H^+ + NH_3$	$\longrightarrow$	$NH_3^+ + H$	[1,10]
$H_2^+ + NH_3$	$\longrightarrow$	$NH_3^+ + H_2$	[1,10]
$H_2^+ + N_2$	$\longrightarrow$	$N_2H^+ + H$	[1,10]
$H_3^+ + N$	$\longrightarrow$	$NH_2^+ + H$	[1,10]
$H_3^+ + NH_3$	$\longrightarrow$	$NH_4^+ + H_2$	[1,10]
$N + H + M$	$\longrightarrow$	$NH + M$	[11]
$NH + NH$	$\longrightarrow$	$N + NH_2$	[11,12]
$NH + NH_2$	$\longrightarrow$	$N + NH_3$	[11,12]
$H + NH_2 + M$	$\longrightarrow$	$M + NH_3$	[11,13]
$H_2 + NH_2$	$\longrightarrow$	$H + NH_3$	[11,13]
$H_2 + NH + M$	$\longrightarrow$	$M + NH_3$	[11,14]
$H_3^+ + N_2$	$\longrightarrow$	$N_2H^+ + H_2$	[1,10]
$N^+ + H_2$	$\longrightarrow$	$NH^+ + H_2$	[1,10]
$N^+ + NH_3$	$\longrightarrow$	$NH_2^+ + NH$	[1,10]
$N^+ + NH_3$	$\longrightarrow$	$NH_3^+ + N$	[1,10]
$N^+ + NH_3$	$\longrightarrow$	$N_2H^+ + H_2$	[1,10]
$NH^+ + H_2$	$\longrightarrow$	$H_3^+ + N$	[1,10]
$NH^+ + H_2$	$\longrightarrow$	$NH_2^+ + H$	[1,10]
$NH^+ + NH_3$	$\longrightarrow$	$NH_3^+ + NH$	[1,10]
$NH^+ + NH_3$	$\longrightarrow$	$NH_4^+ + N$	[1,10]
$NH^+ + N_2$	$\longrightarrow$	$N_2H^+ + N$	[1,10]
$NH^+ + H_2$	$\longrightarrow$	$NH_3^+ + H$	[1,10]
$NH_2^+ + NH_3$	$\longrightarrow$	$NH_3^+ + NH_2$	[1,10]
$NH_2^+ + NH_3$	$\longrightarrow$	$NH_4^+ + NH$	[1,10]
$NH_3^+ + NH_3$	$\longrightarrow$	$NH_4^+ + NH_2$	[1,10]
$N_2^+ + H_2$	$\longrightarrow$	$N_2H^+ + H$	[1,10]
$N_2H^+ + NH_3$	$\longrightarrow$	$NH_4^+ + N_2$	[1,10]

$N_2^+ + NH_3$	$\longrightarrow$	$NH_4^+ + N_2$	[1,10]
$N_2^+ + H_2O$	$\longrightarrow$	$H_2O^+ + N_2$	[4,15]
$OH^- + NO_2$	$\longrightarrow$	$NO_2^- + OH$	[4,15]
$e + NO_3 + M$	$\longrightarrow$	$M + NO_3^-$	[4,16]
$e + H_2O$	$\longrightarrow$	$H + OH^-$	[4]
$e + NO_2 + M$	$\longrightarrow$	$M + NO_2^-$	[4,16]
$e + N_2^+ + M$	$\longrightarrow$	$M + N_2$	[4,17]
$O + O + M$	$\longrightarrow$	$M + O_2$	[4,18]
$H^- + H$	$\longrightarrow$	$H_2 + e$	[4,19]
$OH^- + O$	$\longrightarrow$	$HO_2 + e$	[4,15]
$OH^- + H$	$\longrightarrow$	$H_2O + e$	[4,19]
$N + OH$	$\longrightarrow$	$NO + H$	[4,15]
$N + HO_2$	$\longrightarrow$	$NO + OH$	[4,15]
$OH + OH$	$\longrightarrow$	$H_2O + O$	[4,15]
$OH + HO_2$	$\longrightarrow$	$H_2O + O_2$	[4,20]
$OH + H_2$	$\longrightarrow$	$H_2O + H$	[4,15]
$O + H + M$	$\longrightarrow$	$M + OH$	[4,21]
$N + O + M$	$\longrightarrow$	$M + NO$	[4,18]
$H + H + M$	$\longrightarrow$	$M + H_2$	[4,22]
$OH + H + M$	$\longrightarrow$	$H_2O + M$	[4,22]
$OH + OH + M$	$\longrightarrow$	$H_2O_2 + M$	[4,21]
$N + N + M$	$\longrightarrow$	$N_2 + M$	[4,15]
$N + O_3$	$\longrightarrow$	$NO + O_2$	[4,23]
$e + O_2 + O$	$\longrightarrow$	$O_2 + O^-$	[4]
$NO_3 + O^-$	$\longrightarrow$	$NO_2^- + O^-$	[4,16]
$NO_2^- + NO_2$	$\longrightarrow$	$NO_3^- + NO$	[4,15]
$NO_2^- + NO_3$	$\longrightarrow$	$NO_3^- + NO_2$	[4,15]
$N + O + M$	$\longrightarrow$	$O_3 + M$	[4,18]
$O + O_2 + M$	$\longrightarrow$	$O_3 + M$	[4,18]
$N + O_2$	$\longrightarrow$	$NO + O$	[4,17]
$O + NO + M$	$\longrightarrow$	$NO_2 + M$	[4,18]
$NO + O_3$	$\longrightarrow$	$NO_2 + O_2$	[4,18]
$NO_2 + O_3$	$\longrightarrow$	$NO_3 + O_2$	[4,18]
$OH + NO + M$	$\longrightarrow$	$HNO_2 + M$	[4,18]
$HNO_2 + H$	$\longrightarrow$	$NO_2 + H_2$	[4,18]
$HO_2 + NO$	$\longrightarrow$	$OH + NO_2$	[4,21]
$HNO_2 + HNO_2$	$\longrightarrow$	$NO_2 + H_2O + NO$	[4,16]
$H + Sur$	$\longrightarrow$	$H(s)$	[1]
$N + Sur$	$\longrightarrow$	$N(s)$	[1]
$NH + Sur$	$\longrightarrow$	$NH(s)$	[1]
$NH_2 + Sur$	$\longrightarrow$	$NH_2(s)$	[1]
$N + H(s)$	$\longrightarrow$	$NH(s)$	[1]
$N(s) + H$	$\longrightarrow$	$NH(s)$	[1]
$H_2 + NH(s)$	$\longrightarrow$	$NH_3 + Sur$	[1]
$NH + H(s)$	$\longrightarrow$	$NH_2(s)$	[1]
$H + NH_2(s)$	$\longrightarrow$	$NH_3 + Sur$	[1]

$NH_2 + H(s)$	$\longrightarrow$	$NH_3 + Sur$	[1]

Table S2: Concentration of reactive species at point C of 1D model (Figure 7) after 1000 s simulation.

Reactive species	Relative concentration (mol/m^3)
N	0.03
H	1.62 X10^{-14}
O	2.86 X10^{-17}
OH	6.67 X10^{-25}
H_2O_2	5.99 X10^{-14}
NO	4.31X10^{-7}
NO_2	3.73 X10^{-18}
NO_3	9.74 X10^{-21}
NO_3^-	1.31 X10^{-15}
NO_2^-	6.57 X10^{-12}
NH_3	2.50 X10^{-18}
NH_4^+	8.54 X10^{-11}
NH	2.66 X10^{-10}

Energy consumption for total N-fixation (NO_3^- + NH_4^+)

$$EC\left(\frac{MJ}{mol}\right) = \frac{Power}{Moles\left[NO_3^- + NH_4^+\right]per\ second\ \left[mol.s^{-1}\right]} \times \frac{1}{10^6\ [\frac{J}{MJ}]}$$

EC for total N-fixation = 12 MJ/mol

Energy consumption for NO_3^--fixation

$$EC\left(\frac{MJ}{mol}\right) = \frac{Power}{Moles\left[NO_3^-\right]per\ second\ \left[mol.s^{-1}\right]} \times \frac{1}{10^6\ [\frac{J}{MJ}]}$$

EC for NO_3^- = 41 MJ/mol

Energy consumption for NH_4^+-fixation

$$EC\left(\frac{MJ}{mol}\right) = \frac{Power}{Moles\left[NH_4^+\right]per\ second\ \left[mol.s^{-1}\right]} \times \frac{1}{10^6\ [\frac{J}{MJ}]}$$

EC for NH_4^+ = 17 MJ/mol

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