Supplementary Information

Hydrogen Release Mechanism for Hydrolysis of Ammonia Borane over Pd/C_3N_4 Nanocatalyst Synthesized by Electron Beam Irradiation

Manish Shingole[1], Seemita Banerjee*[1,2], Priyanka Ruz[2], Asheesh Kumar[2], Pratibha Sharma[3], V. Sudarsan[1,2]

[1]Homi Bhabha National Institute, Mumbai India

[2]Chemistry Division, Bhabha Atomic Research Centre, Mumbai, India

[3]Department of Energy Science and Engineering, IIT Bombay, Powai, Mumbai, India

*Corresponding Author Email: seemita@barc.gov.in

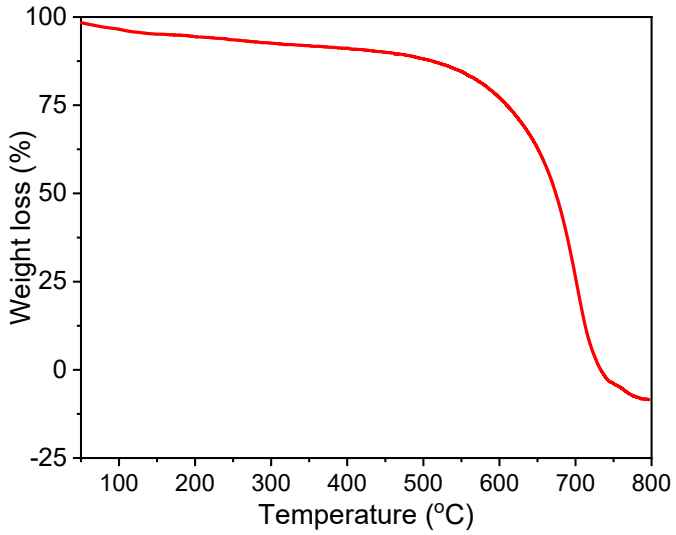
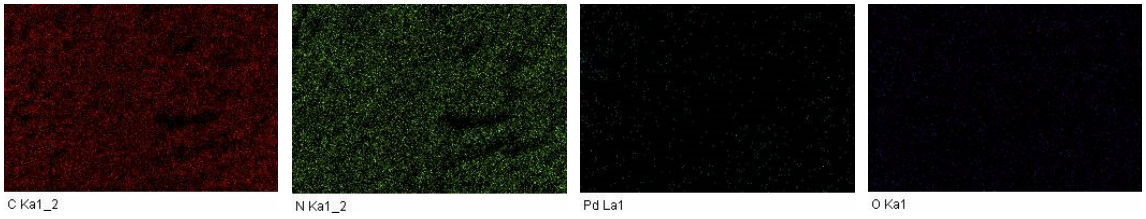
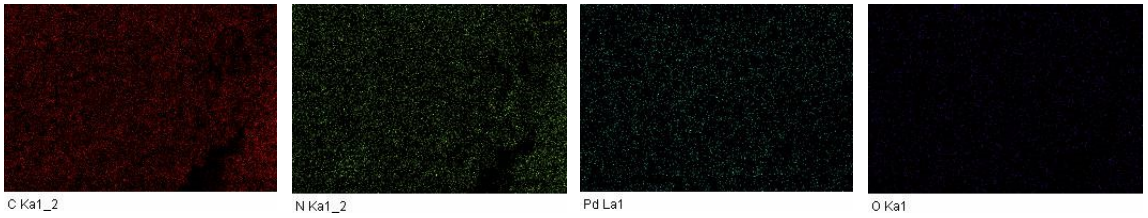


Figure S1: TGA curves of ex-C_3N_4 in air at a heating rate of 10 K min^{-1}, using Setsys Evolution, SETARAM, France

.

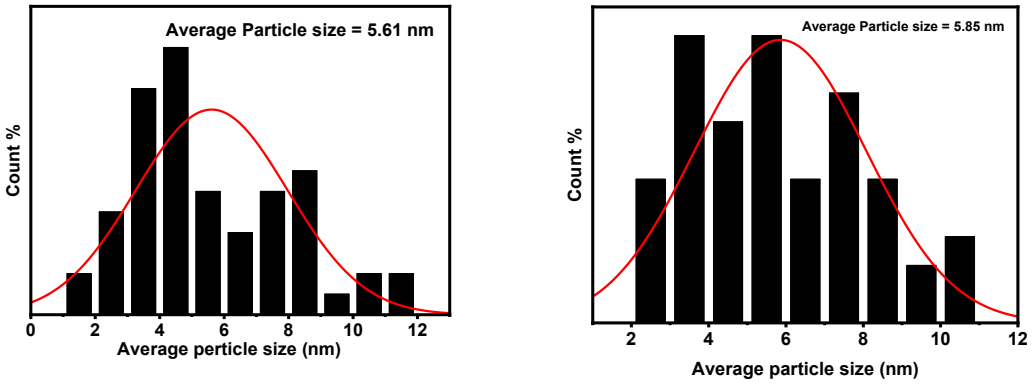


(a)



(b)

Figure S2: Elemental mapping of C, N, Pd, and O of (a) CNPd1 and (b) CNPd5



(a) (b)

Figure S3: Particle size distribution of Pd nanoparticles in (a) CNPd1 (b) CNPd5

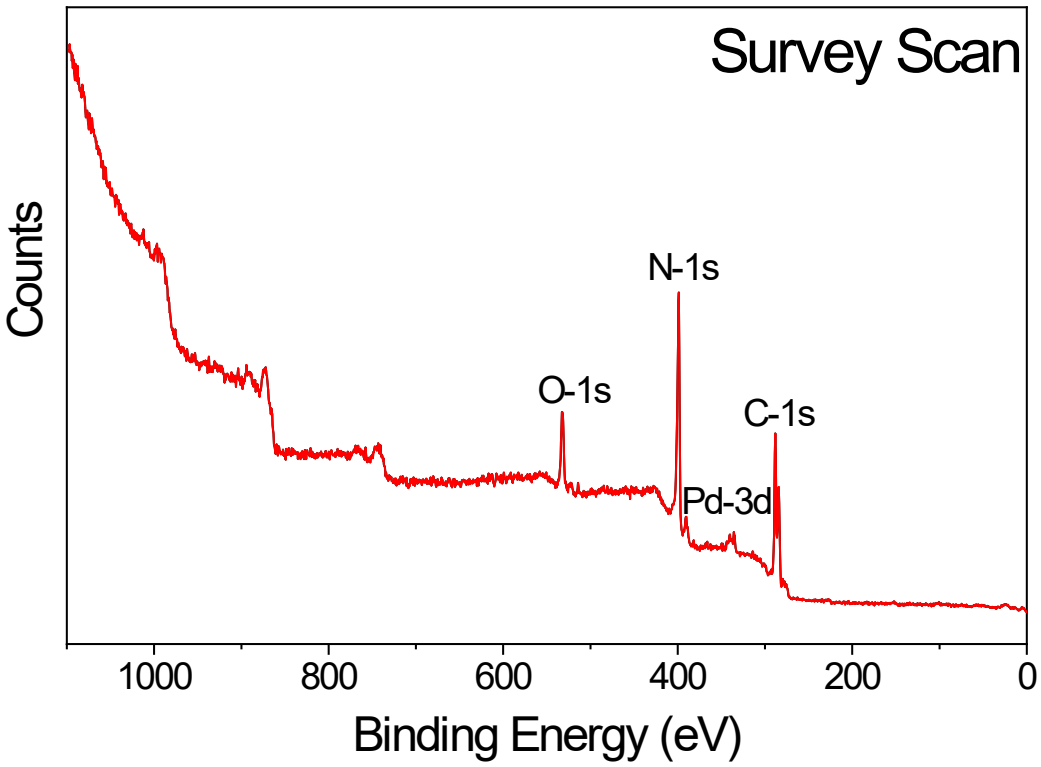
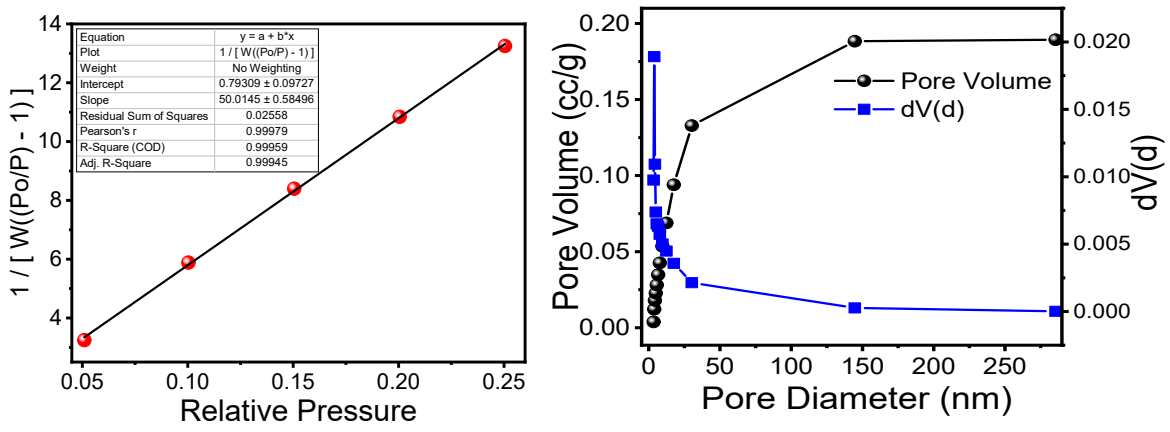
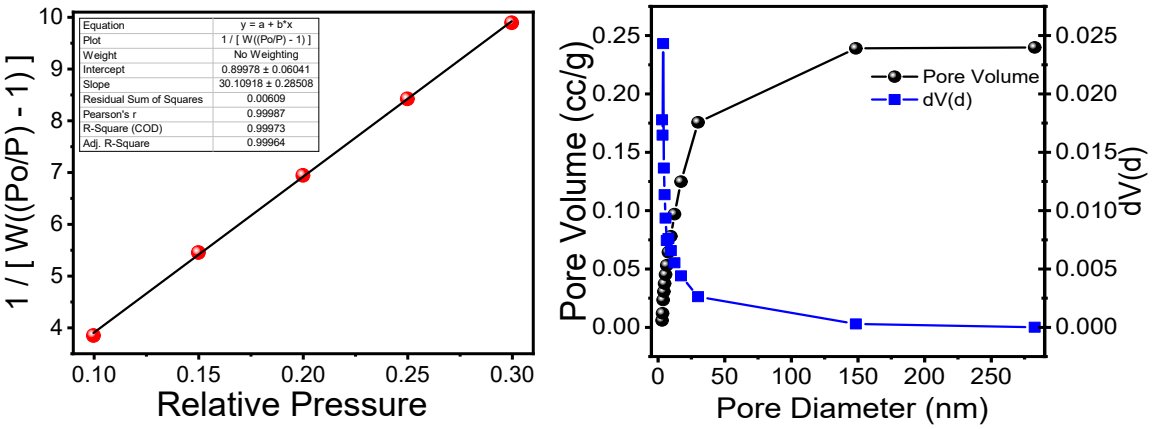


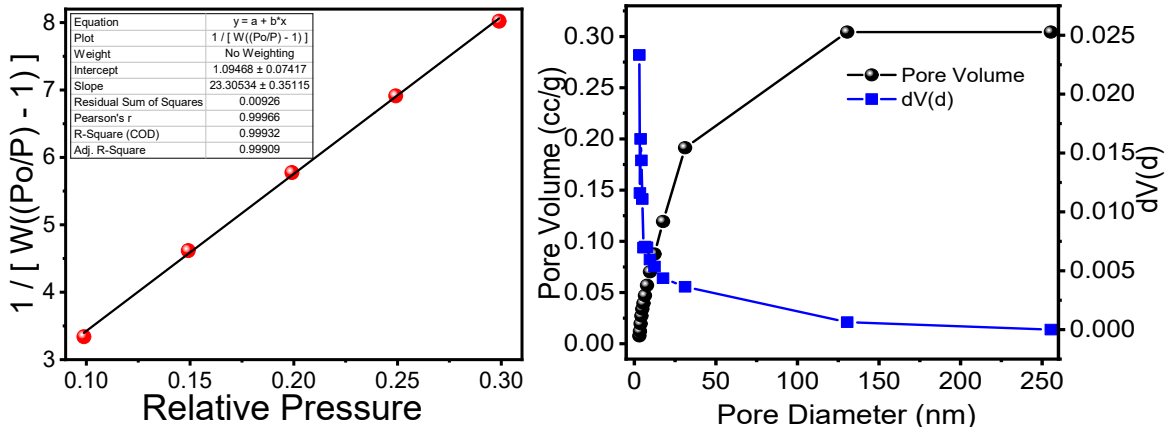
Figure S4: XPS survey scan of CNPd5



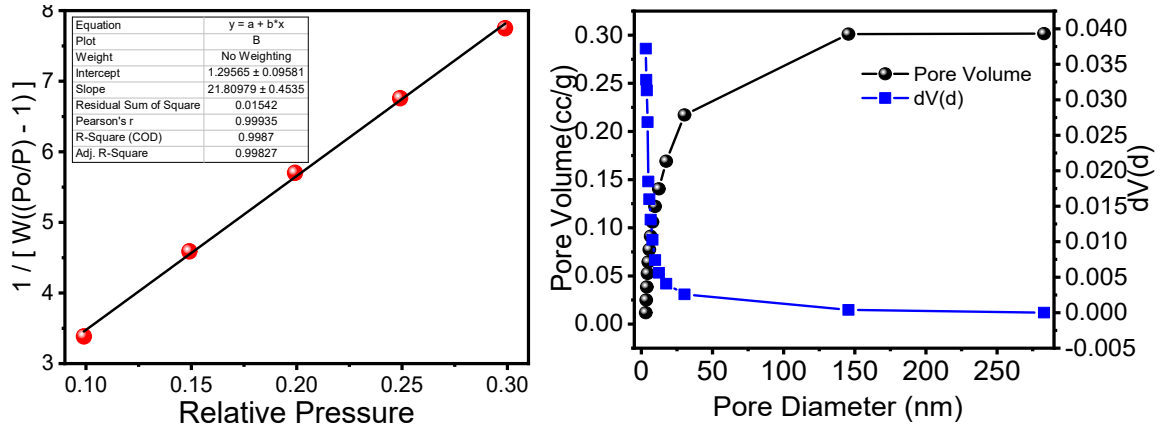
(a) C_3N_4



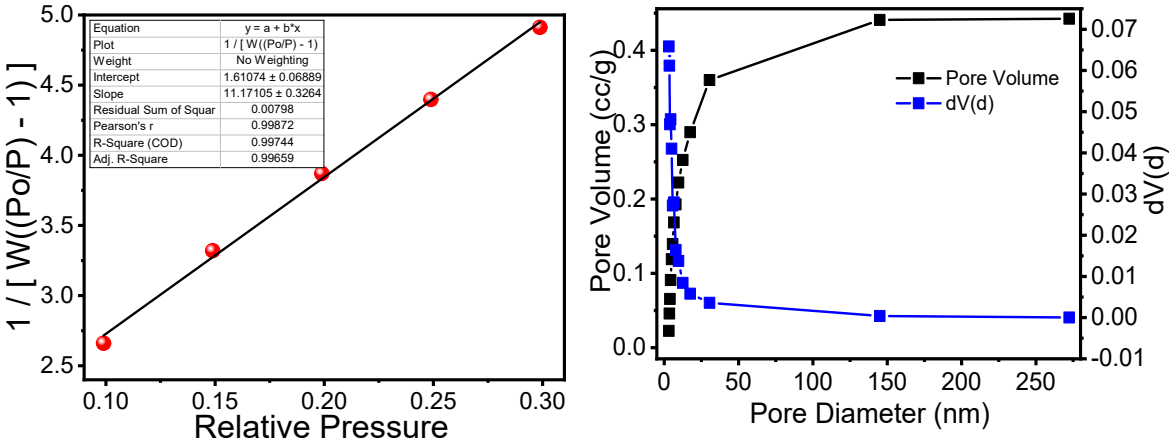
(b) Ex-C_3N_4



(c) CNPd1



(e) CNPd3



(f) CNPd5

Figure S5 BET plot for surface area analysis and BJH pore size distribution of the samples

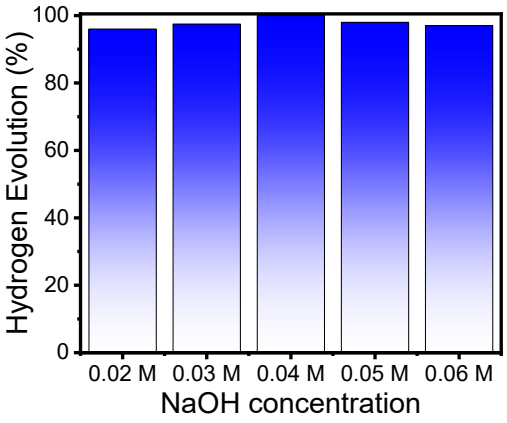


Figure S6 Optimization of the NaOH concentration for the Hydrogen evolution from the CNPd5 catalysed AB hydrolysis

Table S1: Activation energy for the ammonia borane hydrolysis reaction in presence of supported Pd catalyst (NA-Not Available)

Entry	Catalyst	Activation Energy (kJ/mol)	TOF (min^{-1})	Pd particle size (nm)	References
1	Pd/C_3N_4	27.36	38.2	5.85	This Study
2	Pd^0/CeO_2	68	29	2-6	1
3	RGO@Pd	38	26.3	5	2
4	Pd(0)-HAP	55	NA	3.6	3
5	Pd-PVB-TiO_2	55.9	NA	NA	4
6	Pd/Co_3O_4	62	3048	2.6	5
7	Pd/PDA- $CoFe_2O_4$	65	175	2.7	6
8	Pd/α-LDH	20	49.5	5.6	7
9	Pd/MCN	57	125	2.7	8
10	Pd/IPCNs	29.1	122.8	2.17	9
11	$Pd/Fe_3O_4@SiO_2$-PC	28.4	47.3	2.3	10
12	Pd/CS-rGO	39	42.5	1.7	11
13	Pd/C	67.5	40	3.6	12
14	Pd(0)/g-C_3N_4-CS	35.3	25.3	1.4	13
15	Pd/CGP-GO-Fe_3O_4	36.5	16.2	NA	14
16	Pd/PDA-Fe3O4	65	14.5	2	15
17	RGO-Pd	51	6.25	4	16
18	CuFe2O4–NH2@Pd	38.54	NA	3-5	17
19	PdCo@NCHP	36.9	470.5	NA	18

20	Ni−MoO_x	NA	85.7	3	19
21	CoCu	38.6	11.56	8.6	20
22	CuNi	23.58	2.08	3.9	21
23	RuNi	27.2	905	1.40	22
24	RuCo	22.5	139	1.56-2.94	23

References for Supplementary Information

1. Y. Tonbul, S. Akbayrak and S. Özkar, *international journal of hydrogen energy*, 2016, **41**, 11154-11162.
2. B. Kılıç, S. Şencanlı and Ö. Metin, *Journal of Molecular Catalysis A: Chemical*, 2012, **361**, 104-110.
3. M. Rakap and S. Özkar, *international journal of hydrogen energy*, 2011, **36**, 7019-7027.
4. M. Rakap, E. E. Kalu and S. Özkar, *international journal of hydrogen energy*, 2011, **36**, 1448-1455.
5. S. Akbayrak, Z. Özçifçi and A. Tabak, *Journal of colloid and interface science*, 2019, **546**, 324-332.
6. J. Manna, S. Akbayrak and S. Özkar, *Applied Catalysis B: Environmental*, 2017, **208**, 104-115.
7. Y. H. Zhou, S. Wang, Z. Zhang, N. Williams, Y. Cheng and J. Gu, *ChemCatChem*, 2018, **10**, 3206-3213.
8. W. Wang, Z. H. Lu, Y. Luo, A. Zou, Q. Yao and X. Chen, *ChemCatChem*, 2018, **10**, 1620-1626.
9. M. Mao, Q. Chen, J. Wu and G. Fan, *International Journal of Hydrogen Energy*, 2020, **45**, 27244-27253.
10. S. Liu, Y.-T. Li, X.-C. Zheng, X.-X. Guan, X.-L. Zhang and P. Liu, *International Journal of Hydrogen Energy*, 2020, **45**, 1671-1680.
11. S. Liu, X. Chen, Z.-J. Wu, X.-C. Zheng, Z.-K. Peng and P. Liu, *International Journal of Hydrogen Energy*, 2019, **44**, 23610-23619.
12. S. Akbayrak and S. Özkar, *Journal of Colloid and Interface Science*, 2022, **626**, 752-758.
13. H. Jia, X. Chen, X. Song, X. Zheng, X. Guan and P. Liu, *International Journal of Energy Research*, 2019, **43**, 535-543.
14. H. Jia, S. Liu, G.-P. Zheng, X.-C. Zheng, X.-Y. Wang and P. Liu, *International Journal of Hydrogen Energy*, 2019, **44**, 27022-27029.
15. J. Manna, S. Akbayrak and S. Özkar, *RSC advances*, 2016, **6**, 102035-102042.
16. P. Xi, F. Chen, G. Xie, C. Ma, H. Liu, C. Shao, J. Wang, Z. Xu, X. Xu and Z. Zeng, *Nanoscale*, 2012, **4**, 5597-5601.
17. J. Ma, X. Guo and X. Ji, *International Journal of Hydrogen Energy*, 2024, **51**, 345-356.
18. J. Deng, X. Zhou, J. Zou, Y. Qin and P. Wang, *ACS Applied Energy Materials*, 2022, **5**, 7408-7419.
19. W. Liu, L. Yao, X. Sun, W. Wang, G. Feng, Q. Yao, L. Zhang and Z. H. Lu, *ChemSusChem*, 2024, **17**, e202400415.
20. J. Liu, B. Li, Y. Dong, Q. Liu, Y. Song, Y. Guo, Y. Zhao, X. Li and J. Xiong, *Catalysis Letters*, 2024, **154**, 461-472.
21. R. Jiang, M. Yang, J. Meng, P. Zhao, P. Liu and X. Zheng, *International Journal of Hydrogen Energy*, 2023, **48**, 18245-18256.
22. Y. Li, Q. Liu, J. Meng, Y. Yang, Z. Peng and X. Zheng, *Applied Surface Science*, 2022, **605**, 154709.
23. Y. He, Z. Wang, M. Mao, Q. Li and G. Fan, *New Journal of Chemistry*, 2021, **45**, 14759-14764.