Supplementary Information for

Catalyst Screening for Electrochemical Ammonia Synthesis: A Review

Dominik G. Jammal*[1], **Ricardo Bernardino**[1], **Nuno Canha**[1] **Cristina M. Cordas**[1, 2], **Rui P.P.L. Ribeiro**[1, 2]

[1] HyLab- Green Hydrogen Collaborative Laboratory Sines Central Termoelétrica, Estrada Nacional 120-1, 7520-089, Sines, Portugal
[2] LAQV-Requimte, Department of Chemistry, NOVA School of Science and Technology, NOVA University of Lisbon, Caparica, Portugal

* Correspondence: dominik.jammal@hylab.pt

Supporting Information – Selection of Catalytic Systems

The 215 catalytic systems analyzed in this review were systematically compiled from recent review articles to ensure comprehensive and up-to-date coverage of Lithium-mediated, electrochemical, and photo(electro)catalytic nitrogen reduction reactions. The following review publications served as the primary sources for the initial compilation of catalytic systems.[1 – 7] Each system extracted from these reviews was cross-checked against the original primary literature referenced in the respective tables to verify reported performance metrics, including NH_3 production rates, Faradaic efficiencies, and, where available, catalyst costs. Only systems with consistent and verifiable data were included to ensure reproducibility and reliability.

Table S 1: *Comprehensive Overview of 215 Catalytic Systems for N_2 Reduction: Production Rates (PR), Faradaic Efficiencies (FE), Catalyst Costs (CC), and combined Performance Scores.*

	Catalysts	PR (normalized)	FE (normalized)	Costs	Sum of Points	Review Source
1	**Mo foil**	0.53	1.68	5.13	7.3	1
2	**Mo rod**	n/a	1.45	8.44	9.9	1
3	**Cu foil**	0.8	2.71	9.83	13.3	1
4	**steel cloth**	2	4.15	9.89	16.0	1
5	**Au-coated carbon paper**	0.57	4.15	0.5	5.2	1
6	**SSC**	n/a	6.49	9.89	16.4	1
7	**Steel cloth**	0.5	4.56	9.89	15.0	1
8	**Ag wire**	0.56	1.75	8.09	10.4	1
9	**Cu wire**	0.51	6.04	9.85	16.4	1
10	**Mo foil**	0.57	4.33	9.66	14.6	1

11	**Mo foil**	0.56	4.33	9.66	14.6	1
12	**Ni wire**	0.62	9.1	9.77	19.5	1
13	**Ni wire**	0.61	10	9.77	20.4	1
14	**Mo foil**		3.52	9.66	13.2	2
15	**Ni wire**	7	9.91	9.77	26.7	2
16	**Ni wire**	10	9.64	9.77	29.4	2
17	**Cu(HBT)**	1.5	7.57	7.23	16.3	2
18	**Mo foil**	n/a	6.04	9.66	15.7	2
19	**Mo foil**	n/a	8.11	9.66	17.8	2
20	**Mo foil**	0.58	4.6	9.66	14.8	2
21	**Cu (HBT)**	0.55	2.35	7.23	10.1	2
22	**Cu**	3	7.21	9.85	20.1	2
23	**Mo foil**		8.02	9.66	17.7	2
24	**Cu wire**	0.7	4.78	9.85	15.3	2
25	**Fe**	0.52	6.22	9.88	16.6	2
26	**Hollow Cr_2O_3 microspheres**	3.55	1.16	9.84	14.55	3
27	**TiO_2-GO**	2.31	0.76	9.98	13.05	3
28	**Fe_2O_3 nanorods**	2.41	0.5	9.95	12.86	3
29	**Defect-rich MoS_2 nanoflower**	4.03	1.33	9.98	15.34	4
30	**Mo_2C/NC**	10	1.78	9.2	20.98	4
31	**V_2CTx MXene**	2	0.88	2.55	5.43	4
32	**NC/BiSAs/TiN/CC**	9.73	3.17	9.74	22.64	4
33	**JUC-1000**	10	1.74	7	18.74	5
34	**Defective UiO-66-NH2**	6.89	10	9.99	26.88	5
35	**HT AU@MOF**	5.98	7.26	9.48	22.72	5
36	**MoS2@ZIF-71**	1.92	3.88	8.76	14.56	5
37	**Bi_2V_0.1O_x/CeO_2**	3.29	1.54	9.98	14.81	3
38	**B_4C**	3.7	2.19	9.99	15.88	3
39	**Nb_2O_5 nanofiber**	5.78	1.44	9.95	17.17	3
40	**Cr_2O_3/CPE**	3.9	1.36	9.9	15.16	4
41	**TA-reduced Au/TiO_2**	3.08	1.31	7.57	11.96	4
42	**α-Au/CeO_2-RGO**	1.49	1.53	7.13	10.15	3
43	**Au flowers**	3.58	1.08	9.58	14.24	3
44	**Mo_2C@3DUM-C**	4.18	1.46	9.8	15.44	4
45	**Au/Ti_3C_2**	4.19	2.46	7.41	14.06	4
46	**1T-MoS_2/Ti_3C_2**	4.9	0.99	9.57	15.46	4
47	**Cr_3C_2@CNFs**	3.38	1.36	9.99	14.73	4
48	**Ti_3C_2Tx (T_{14}F,OH) MXene nanosheets**	2.96	1.44	7.52	11.92	4

49	**Fluorine-free Ti_3C_2Tx ($T_{14}O$,OH)**	4.96	1.42	9.8	16.18	4
50	**TiO_2/Ti_3C_2Tx**	3.67	1.34	2.5	7.51	4
51	**Hydroxyl-rich Ti_3C_2Tx QDs**	8.11	1.89	2.55	12.55	4
52	**Oxygen-vacancy-rich TiO_2/Ti_3C_2Tx**	4.37	2.21	6.45	13.03	4
53	**Fe-TCPP**	3.91	2.22	9.38	15.51	5
54	**OPA-PCN-222(Fe)**	1.61	2.33	6.94	10.88	5
55	**Mo_2N Nanorods**	10	0.9	8.6	19.5	4
56	**β-FeOOH nanorods**	3.31	1.15	9.99	14.45	3
57	**Mo_2C/C**	1.85	1.27	9.95	13.07	4
58	**Mo_3Fe_3C**	10	3.44	8.9	22.34	4
59	**Co3HHTTP2**	3.16	0.77	9.5	13.43	5
60	**M@ZIF-Oam**	7.37	5.35	9.5	22.22	5
61	**a-FeB2 PNSs**	5.32	2.28	8.29	15.89	
62	**Ni nanoparticles/V_4C_3Tx MXene**	3.06	2.07	2.55	7.68	4
63	**W_2N_3**	1.89	1.71	9.47	13.07	4
64	**Ti_3C_2 MXene nanoribbons**	2.27	0.74	2.5	5.51	4
65	**Cu@Ce-MOF-2**	5.92	1.61	9.57	17.1	5
66	**Co3Fe-MOF**	6.5	3.28	0.5	10.28	5
67	**Au nanorods**	0.67	0.83	9.93	11.43	3
68	**γ-Fe_2O_3**	0.5	0.61	10	11.11	3
69	**NeS-doped Ti_3C_2Tx**	4.64	1.14	8.11	13.89	4
70	**N-doped porous carbon**	3.37	0.55	8.92	12.84	3
71	**CNT@CAU-17**	2.09	3.92	6.21	12.22	5
72	**Co-TCPP**	2.86	1.69	9.78	14.33	5
73	**Zn-TCPP**	6.52	1.11	6.95	14.58	5
74	**NiFe-MOF**	1.55	1.69	6.95	10.19	5
75	**NCNT@CAU-17**	0.93	2.64	9.66	13.23	5
76	**CNT@UIO-66**	1.22	2.1	9.66	12.98	5
77	**NCNT@UIO-66**	0.97	2.44	8.24	11.65	5
78	**CNT@BIT-58**	1.47	1.79	8.24	11.5	5
79	**NCNT@BIT-58**	1.14	2.08	1.84	5.06	5
80	**NCNT@MIL-101(Fe)**	1.32	3.23	1.84	6.39	5
81	**CNT@MIL-101(Fe)**	3.6	4.6	8.29	16.49	5
82	**TiO_2/Ti**	0.979	0.98	9.92	11.879	3
83	**MoS_2/CC**	0.92	0.69	9.82	11.43	3
84	**MnO/TM**	1.08	2.18	10	13.26	4
85	**Fe_3O_4/Ti**	0.5	1	9.91	11.41	3

86	**a-Mo_2C**	10	9.12	9.94	29.06	4
87	**TiN-PE**	2.24	2.4	9.61	14.25	4
88	**ZIF-67@Ti3C2**	10	4.8	2.13	16.93	5
89	**In-MOF**	1.86	3.69	8.6	14.15	5
90	**H-KUST**	0.89	0.97	5.25	7.11	5
91	**MoO_3 nanosheet**	3.01	0.85	9.52	13.38	3
92	**Mo nanofilm**	0.7	0.59	9.88	11.17	3
93	**Ru/C**	0.51	0.5	9.52	10.53	3
94	**VN/TM**	0.93	0.92	8.91	10.76	3
95	**Ag nanosheet**	0.74	1.48	9.86	12.08	3
96	**MoN**	0.51	0.68	7.64	8.83	3
97	**MoN NA/CC**	2.07	0.68	0.76	3.51	4
98	**TiB2**	1.41	2.91	9.88	14.2	4
99	**VN/CC**	1.79	1.21	6.75	9.75	4
100	**MV-MoN@NC**	7.08	1.93	0.5	9.51	4
101	**Mo_2N**	2.91	1.41	9.85	14.17	4
102	**PEBCD/C**	0.63	1.05	9.6	11.28	3
103	**AuHNCs**	0.83	0.5	8.3	9.63	3
104	**Surface-engineered Ti_3C_2**	0.64	1.96	4.24	6.84	4
105	**NH2–MIL-88B–Fe**	1.13	3.14	0.5	4.77	3
106	**Au nanorod**	0.51	1.3	9	10.81	3
107	**Ru/Ti**	1.12		8.7	9.82	3
108	**VN**	2.23	1.74	8.93	12.9	4
109	**Cu/Ti_3C_2Tx MXene**	10	2.02	8.43	20.45	4
110	**Ag-Au@ZIF**	0.55	4.35	7.75	12.65	5
111	**CrO0.66N0.56**	0.96	1.93	7.5	10.39	4
112	**Au@ZIF-8**	2.96	10	6.6	19.56	5
113	**Fe_2O_3–CNT**	0.51	0.47	0.5	1.48	3
114	**CP_2TiCl_2**	5.48	0.48	9.86	15.82	3
115	**Fe-BiOBr nanosheet (1)**	6.36	0.44	9.99	16.79	6
116	**Fe-BiOCl nanosheet (2)**	8.4	2.67	9.99	21.06	6
117	**Bi5O7Br nanotube**	8.16	3.29	9.99	21.44	6
118	**Bi2MoO6 sphere**	8.17	1.34	9.98	19.49	6
119	**CuCr-LDH nanosheet**	2.41	0.98	9.98	13.37	6

120	**MoO3−x nanosheet**	6.11	0.82	9.51	16.44	6
121	**Ti3C2Tx/TiO2**	6.49	0.5	9.6	16.59	6
122	**WO3**	4.09	0.59	9.98	14.66	6
123	**P-C3N4**	1.6	1.68	10	13.28	6
124	**Au-Ru$_{0.31}$ Nanokristalle**	3.43	0.7	7.83	11.96	6
125	**Mo-$W_{18}O_{49}$ Ultrathin Nanowires**	5.16	0.85	9.94	15.95	6
126	**Au/TiO_2-OV**	4.54	1.46	9.72	15.72	6
127	**CuCr-LDH Nanosheets**	2.79	0.56	9.98	13.33	6
128	**SAFe-porous g-C_3N_4**	2.51	0.56	9.95	13.02	7
129	**Co-doped Bi_2MoO_6**	3.37	1.7	9.37	14.44	7
130	**Fe/Zr-MOFs**	2.27	1.13	9.39	12.79	7
131	**COFX Au**	6.66	0.8	9.33	16.79	6
132	**Ru/MOF/C_3N_4**	9.99	10	8.42	28.41	6
133	**PCN-V**	0.88	1.68	9.98	12.54	6
134	**IN2S3-X@ZnS**	2.53	0.57	9.63	12.73	6
135	**Ag-Pt/TiO2**	1.87	0.59	9.69	12.15	6
136	**POM(PMo10V2) and MOF(MIL-88-A)**	2.3	0.8	9.94	13.04	6
137	**CEF3/LiNbO3**	2.94	0.82	9.66	13.42	6
138	**Ru-KzTa2O6-x**	1.24	1.38	8.44	11.06	6
139	**C3N4/MoS2/Mn3O4 SVs**	5.03	1.93	9.71	16.67	6
140	**B-C3N4 (MoO2)**	8.2	1.21	9.97	19.38	6
141	**Au/TiO2**	2.96	1.46	9.72	14.14	6
142	**Au/g-C3N4 hollow sphere**	6.45	1.23	9.64	17.32	6
143	**Ru-CoS/g-C3N4 SVs**	6.53	2.02	9.59	18.14	6
144	**BiOBr nanosheet (1)**	2.44	n/a	9.99	12.43	6
145	**Bi5O7Br nanostructure**	10	n/a	9.99	19.99	6
146	**Bi2MoO6/BiOBr**	3.3	n/a	9.97	13.27	6
147	**H-Bi5O7I**	5.5	n/a	9.98	15.48	6
148	**$Cu^{\delta+}$-ZnAl-LDH nanosheet**	3.46	n/a	9.98	13.44	6
149	**FeS2-FeP-CeO2**	9.65	n/a	9.96	19.61	6
150	**In2O3/In2S3 microsphere**	2.08	n/a	9.53	11.61	6
151	**GaN (Ru) NVs**	6.52	n/a	8.5	15.02	6
152	**Ultrathin MoS2 SVs**	6.06	n/a	9.97	16.03	6
153	**FeN-CDs/TiO_2@CN**	6.35	n/a	9.99	16.34	7

154	**Al-PMOF(Fe)**	0.5	n/a	9.98	10.48	7
155	**Pt_1/N-MoS_2**	3.88	n/a	3.26	7.14	7
156	**Fe-BiOCl Nanosheets**	8.4	n/a	9.96	18.36	7
157	**Au/$(BiO)_2CO_3$**	2.03	n/a	9.64	11.67	7
158	**5%Ru@n-GaN NWs**	3.86	n/a	8.3	12.16	7
159	**Cs_2O/Os-Au**	9.61	n/a	0.5	10.11	7
160	**UiO-66(-NH_2)/$CuInS_2$**	7.08	n/a	6	13.08	7
161	**$FeIN_2S_4$/Fe-Pal**	7.56	n/a	9.55	17.11	7
162	**Bi_2S_3/OV-Bi_2MoO_6**	3.91	n/a	9.96	13.87	7
163	**Cu-Cu_2O/CMOH**	5.47	n/a	9.78	15.25	7
164	**Co-doped Bi_2MoO_6 (1)**	4.53	n/a	9.37	13.9	7
165	**Cu-doped Bi_2MoO_6 (2)**	5.63	n/a	9.37	15	7
166	**Bi–MOF/g-C_3N_4**	5.45	n/a	9.99	15.44	7
167	**Cu_2O Clusters/MIL-100(Fe)**	2.33	n/a	9.93	12.26	7
168	**BiOBr/OV-TiO_2-Cu**	5.05	n/a	9.96	15.01	7
169	**S-doped-g-C_3N_4**	9.93	n/a	10	19.93	7
170	**Carbon-$WO_3 \cdot H_2O$**	5.56	n/a	9.98	15.54	7
171	**ZnO/ZnSnO3/Carbon Dots**	9.74	n/a	9.99	19.73	7
172	**TiO2/BiOBr**	8.11	n/a	9.99	18.1	7
173	**Bi2SN2O7/BiOBr**	6.59	n/a	9.98	16.57	7
174	**Boron-doped graphene quantum dots/Bi2MoO6**	5.48	n/a	9.36	14.84	7
175	**2D/2D Bi12O17Br2/ZnCr-LDH**	6.2	n/a	0.85	7.05	7
176	**N-graphyne/Bi/BiOBr**	1.61	n/a	9.87	11.48	7
177	**p-TiO2**	2.63	n/a	10	12.63	7
178	**Bi2S3@PCN**	1.08	n/a	9.98	11.06	7
179	**NanoMIL-125(Ti)**	5.46	n/a	10	15.46	7
180	**COF/g-C3N4/CNT**	5.21	n/a	9.51	14.72	7
181	**NiSnO3-g-C3N4**	7.47	n/a	9.93	17.4	7
182	**Sb/TiO2**	1.33	n/a	9.99	11.32	6
183	**Few-layer g-C3N4 NVs**	9.97	n/a	10	19.97	6
184	**NC-g-C3N4**	8.22	n/a	10	18.22	6
185	**MOF-74(Zn)@DF-C3N4**	8.35	n/a	9.99	18.34	6
186	**S-g-C3N4 nanosheet CVs**	9.93	n/a	9.99	19.92	6

187	**WS2@TiO2 film**	8.18	n/a	9.92	18.1	6
188	**B-g-C3N4 Nanosheet**	6.35	n/a	9.98	16.33	6
189	**B-g-C3N4**	6.5	n/a	9.98	16.48	6
190	**YF3+/ATP nanocomposite**	2.12	n/a	9.65	11.77	6
191	**In(OH)3/g-C3N4**	9.58	n/a	9.65	19.23	6
192	**Fe-SrMoO4**	3.4	n/a	9.93	13.33	6
193	**Cyano group/g-C3N4**	9.49	n/a	9.99	19.48	6
194	**In2S3 nanotube SVs**	2.36	n/a	9.48	11.84	6
195	**Pr3+: CeF3/ATP (attapulgite)**	7.55	n/a	9.82	17.37	6
196	**AuRuNPs**	3.43	n/a	6.96	10.39	6
197	**Bi2O2CO3 nanosheet**	4.67	n/a	9.96	14.63	6
198	**TiO2 nanotubular**	7.29	n/a	9.98	17.27	6
199	**O-g-C3N4 NVs**	9.88	n/a	10	19.88	6
200	**S-g-C3N4 NVs**	3.14	n/a	10	13.14	6
201	**1T-MoS2/CdS SVs**	10	n/a	8.74	18.74	6
202	**Mo0.1Ni0.1Cd0.8S SVs**	2.72	n/a	7.79	10.51	6
203	**Zn0.1Sn0.1Cd0.8S SVs**	3	n/a	6.4	9.4	6
204	**Holey g-C3N4 nanosheet CVs**	6.41	n/a	9.74	16.15	6
205	**g-C3N4/ZnMoCdS SVs**	2.87	n/a	8.47	11.34	6
206	**Sn-doped MOF-5**	5.13	n/a	9.81	14.94	7
207	**TiO2 QDs/ Fe3S4**	9.36	n/a	9.93	19.29	7
208	**g-C3N4/rGO**	4.57	n/a	7.38	11.95	7
209	**Bi2O3/CdMoO4**	3.33	n/a	8.11	11.44	7
210	**g-C3N4/MoS2/PbTiO3**	9.72	n/a	8.97	18.69	7
211	**NaNbO3/Bi2O2CO3**	4.13	n/a	7.85	11.98	7
212	**TiO2 QDsmodified Bi2O3/NaBiS2**	7.12	n/a	9.77	16.89	7
213	**TCN/ZnS/ZnIN2S4**	7.04	n/a	0.5	7.54	7
214	**Ag-δ-Bi_2O_3**	0.5	n/a	7.69	8.19	7
215	**g-C3N4/Ag2CO3 heterojunction NVs**	4.77	n/a	8	12.77	7

S2. Machine Learning Analysis

The Supplementary Information includes the Silhouette plots, Elbow plots, and a parallel coordinates plot that were used to guide the machine learning clustering procedure. The Silhouette and Elbow plots were applied to quantitatively evaluate cluster cohesion and separation, enabling the identification of the optimal number of clusters. The parallel coordinates plot provides a complementary visualization of the multidimensional relationships among the catalytic systems and their performance metrics. Together, these analyses document the methodological steps leading to the final clustering solution and support a clear and transparent interpretation of the machine learning outcomes.

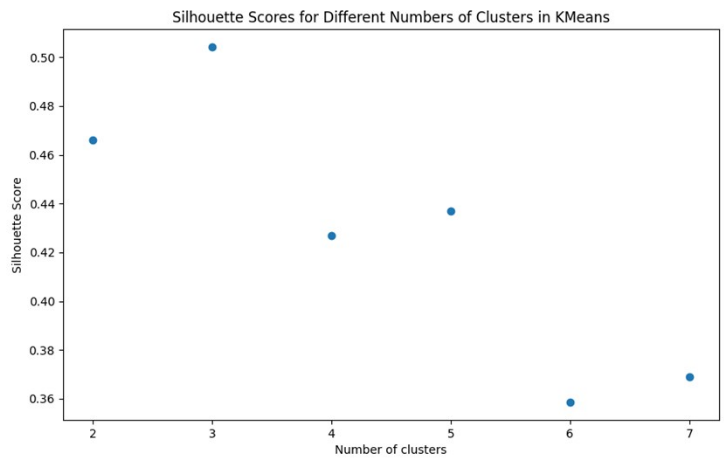

Figure S1: *Silhouette Scores for different numbers of Clusters*

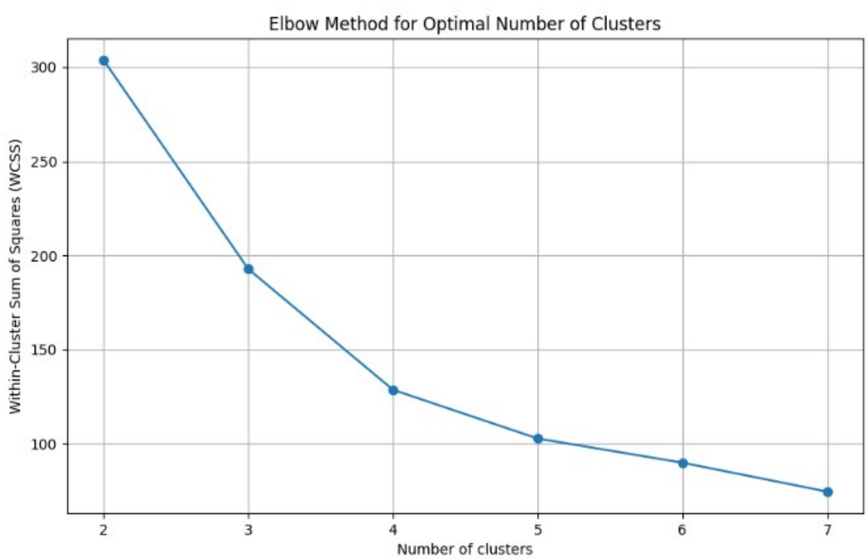

Figure S2: *Elbow Method for Determining the Optimal Number of Clusters*

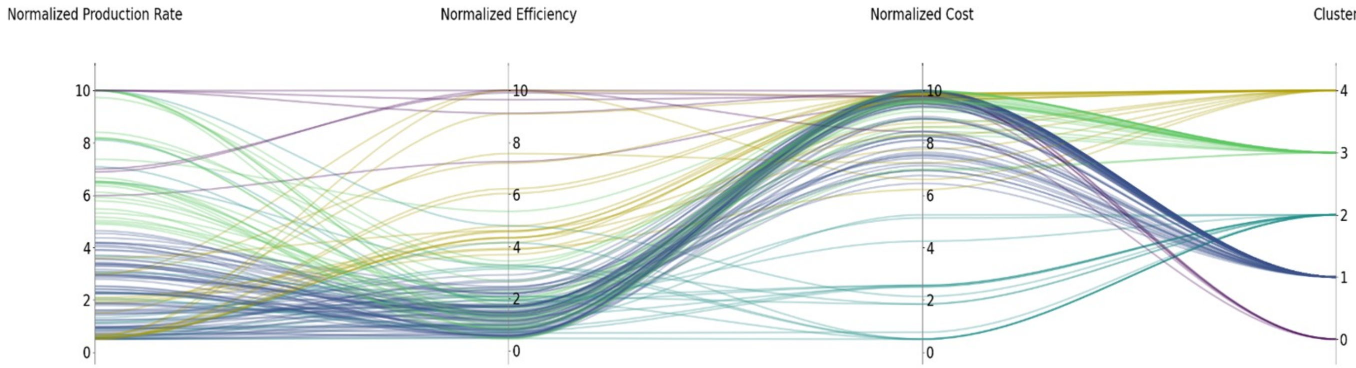

Figure S3: *Visualization of Catalytic Systems Using Parallel Coordinates Plot.*

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